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THEORY AND APPLICATIONS OF SPECTRAL METHODS

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Abstract

An overview of some of the recent major developments in the theory and applications of pseudospectral method is provided. The article is divided into two parts - theory and application to Fluid Dynamics. The part on theory summarizes the results pertaining to the basic principles of pseudospectral methods, their implementation and the relevant error estimates. The part on applications is divided into two sections - incompressible and compressible flows. The section on incompressible flows is confined to the simulation of stability transition and turbulence by spectral methods. The compressible flows section presents a fairly up-to-date review of spectral methods as applied to Potential and Euler equations. The last subsection discusses briefly a spectral algorithm for compressible Navier-Stokes equations.

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INTRODUCTION

The 1977 monograph by Gottlieb and Orszag reviewed the state of the art, at that time, of spectral methods. The theory presented in that work centered on the Galerkin and tau methods and the fluid dynamical applications were confined to incompressible flows. In the past several years, there has been extensive activity both in the theory and application of spectral methods. This activity has been mainly concentrated in the area of pseudospectral methods. For the theory, functional analysis has proved to be a powerful tool for obtaining useful error estimates. For spectral techniques, improved iteration methods have been developed that make possible large-scale calculations of complicated physical phenomena. For applications, first results for compressible flow problems have been obtained for rather complicated flow fields including shock waves and significant progress has been made on transition and turbulence in incompressible flows.

The aim of this article is to review some of the major developments that were made since 1977. We concentrate on pseudospectral techniques as the analysis of Galerkin and tau methods is adequately covered in our 1977 monograph. The review is divided into two main parts. First, we give a summary of results that explain the nature of pseudospectral methods, the correct way to implement them, and the error behavior that should be expected to be produced by them. It should be noted that some very important results in the theory of spectral methods are omitted. Our guideline has been to quote those results that are used in the applications discussed in the second part.

The part on applications contains two major subsections, namely incompressible and compressible flows. Our review is by no means exhaustive: some major applications are not discussed at all. For example there is a

large and rapidly growing literature on the applications of spectral methods in meteorology (see, e.g., Haltiner and Williams 1980). Our goal here is to introduce the potential user to the range of applications of spectral methods and to the problems encountered in implementing them. Spectral methods provide a very sophisticated tool for scientific computing; as in the case of other sophisticated techniques, they can be dangerous if misused. A properly constructed spectral method can be used to obtain solutions where other numerical techniques fail. However, a poorly designed spectral method may perform much worse than simpler finite difference or finite element techniques. We hope that this review will serve as a useful guide to the proper implementation of spectral methods.

1. PSEUDOSPECTRAL FOURIER METHOD

In order to set the framework for this review, let us begin by explaining how to construct pseudospectral approximations. There are basically two steps to obtain a numerical approximation $u_N(x)$ to a solution $u(x)$ of a differential equation. First, an appropriate finite or discrete representation of the solution must be chosen. This may take the form of an interpolating function between the values $u(x_j)$ at some suitable points x_j or series coefficients in the finite representation

$$u_N(x) = \sum_{k=0}^{N} a_k \phi_k(x)$$

with given expansion functions $\phi_k(x)$. The second step is to obtain equations for the discrete values $u_N(x_j)$ or the coeficients a_k from the original equation. In the case of a differential equation, this second step

involves finding an approximation for the differential operator in terms of the grid point values of u_N or, equivalently, the expansion coefficients.

In pseudospectral Fourier approximation, the problem involves periodic boundary conditions. Thus, all functions appearing in the problem are periodic. Let $f(x)$ be a smoothly differentiable function with period 2π. First, we approximate $f(x)$ by the trigonometric polynomial $P_N f(x)$ that interpolates it at one of the following sets of points

$$x_j = \frac{\pi j}{N} \qquad (j = 0,\cdots,2N-1) \tag{1.1a}$$

$$y_j = \frac{2\pi j}{2N+1} \qquad (j = 0,\cdots,2N) \tag{1.1b}$$

$$z_j = \frac{(2j+1)\pi}{2N} \qquad (j = 0,\cdots,2N-1). \tag{1.1c}$$

As will be explained below, fast Fourier transforms (FFT) play a key role in many applications of spectral methods. Many FFT programs are most efficient when 2^P points are transformed, which is not compatible with (1.1b). In practice, the points (1.1a) are most frequently used. This case is discussed first.

When the collocation points x_j given by (1.1a) are used, the approximation $P_N f(x)$ has the form

$$P_N f(x) = \sum_{j=0}^{2N-1} f(x_j) g_j(x) \tag{1.2}$$

where $g_j(x_k) = \delta_{jk}$ and $g_j(x)$ is a polynomial in the functions $\sin x$, $\cos x$ of degree at most N. The polynomials $g_j(x)$ are given explicitly by

$$g_j(x) = \frac{1}{2N} \sin\left[N(x-x_j)\right] \cot \frac{x - x_j}{2} . \tag{1.3}$$

The fact that $g_j(x)$ is a trigonometric polynomial of degree N follows from the equivalent representation

$$g_j(x) = \frac{1}{2N} \sum_{\ell=-N}^{N} \frac{1}{c_\ell} e^{i\ell(x-x_j)} \tag{1.4}$$

where $c_\ell = 1 \left(|\ell| \neq N\right)$, $c_N = c_{-N} = 2$. Thus we can represent $P_N f(x)$ either as

$$P_N f(x) = \frac{1}{2N} \sum_{j=0}^{2N-1} f(x_j) \sin\left[N(x-x_j)\right] \cot \frac{x - x_j}{2} \tag{1.5}$$

using (1.3) or as

$$\begin{aligned} P_N f(x) &= \sum_{j=0}^{2N-1} f(x_j) \frac{1}{2N} \sum_{\ell=-N}^{N} \frac{1}{c_\ell} e^{i\ell(x-x_j)} \\ &= \sum_{\ell=-N}^{N} \frac{1}{c_\ell} e^{i\ell x} \frac{1}{2N} \sum_{j=0}^{2N-1} f(x_j) e^{-i\ell x_j} \end{aligned} \tag{1.6}$$

using (1.4). Defining

$$a_\ell = \frac{1}{2Nc_\ell} \sum_{j=0}^{2N-1} f(x_j) e^{-i\ell x_j} \tag{1.7}$$

(1.6) becomes

$$P_N f = \sum_{\ell=-N}^{N} a_\ell e^{i\ell x} . \tag{1.8}$$

When applying the pseudospectral Fourier method, either the explicit interpolatory formula (1.5), or the complex-Fourier representation (1.7) - (1.8) may be used.

As outlined above, the next step in the pseudospectral method is to seek equations for an approximate solution u_N to a differential equation whose exact solution is u. The crucial step here is to obtain values for the derivatives $\frac{d^k u_N(x)}{dx^k}$ at the collocation points x_j in terms of the values $u_N(x_j)$. This is done pseudospectrally in two formally equivalent, but computationally distinct, ways.

One way is simply to differentiate (1.5) and to evaluate the resulting expression at the points x_j

$$\frac{d^k u_N(x_j)}{dx^k} = \sum_{n=0}^{2N-1} u_N(x_n) \frac{d^k g_n(x_j)}{dx^k} = (d_k \vec{u})_j \tag{1.9}$$

where D_k is an $2N \times 2N$ matrix with elements

$$(D_k)_{j,n} = \frac{d^k g_n(x_j)}{dx^k}$$

and $\vec{u}$ is the column vector

$$\vec{u} = \begin{pmatrix} u_N(x_0) \\ \vdots \\ u_N(x_{2N-1}) \end{pmatrix} .$$

Explicitly,

$$(D_1)_{jn} = \begin{cases} \frac{1}{2}(-1)^{j+n} \cot \frac{x_j - x_n}{2} & j \neq n \\ 0 & j = n \end{cases} \tag{1.10}$$

$$(D_2)_{jn} = \begin{cases} \frac{1}{2}(-1)^{j+n+1} \dfrac{1}{\sin^2 \dfrac{x_j - x_n}{2}} & j \neq n \\ -\dfrac{2N^2+1}{6} & j = n \end{cases} . \qquad (1.11)$$

More generally

$$D_k = (D_1)^k \qquad (1.12)$$

which easily follows from (1.3) and the properties of $g_j(x)$. Also, since D_1 is a real, antisymmetric matrix we note that D_{2k} is a real, symmetric matrix while D_{2k+1} is a real, antisymmetric matrix.

Computationally, the evaluation of derivatives using (1.9) - (1.12) involves the multiplication of an 2N-component vector $\vec{u}$ by an $2N \times 2N$ matrix, D_k, which typically requires $O(N^2)$ arithmetic operations. However, since the matrix product is actually a convolutional sum, it is possible to use the FFT to evaluate (1.9) - (1.12) in only order N log N operations if N is a highly composite integer (like 2^p or 3^q). Nevertheless direct matrix mulitplication can be quite efficient if N is not too large or a highly parallel computer is used.

On the other hand, it is also possible to evaluate derivatives using (1.7) - (1.8). Indeed, (1.8) gives

$$\frac{d^k u_N}{dx^k}(x_j) = \sum_{|n|<N} (in)^k a_n e^{inx_j}, \qquad (1.13)$$

where a_n is given by (1.7). In this approach, a_n is first evaluated by (1.7) and then derivatives at x_j are evaluated by (1.13). If N is a highly composite integer, the two discrete Fourier transforms (1.7) and (1.13)

can be efficiently evaluated by the FFT algorithm in $O(N \log N)$ operations. Thus, evaluation of derivatives requires just two FFTs together with the complex multiplication by $(in)^k$ in (1.13).

The above discussion concentrated on the use of the points x_j given by (1.1a). Now we summarize the results for the sets of points y_j and z_j given by (1.1b) and (1.1c), respectively. The trigonometric polynomial $Q_N f(x)$ that interpolates the periodic function $f(x)$ at the collocation points $x = y_j$ $(j = 0,\cdots,2N)$ is given by

$$Q_N f(x) = \sum_{j=0}^{2N} f(y_j) h_j(x)$$

where

$$h_j(x) = \frac{1}{2N+1} \sin\left[(N + \tfrac{1}{2})(x-y_j)\right] \frac{1}{\sin \frac{x-y_j}{2}} . \tag{1.14}$$

The kth derivative of $Q_N f$ at the point y_j is

$$\frac{d^k Q_N f}{dx^k}(y_j) = \sum_{n=0}^{2N} f(y_n) \frac{d^k}{dx^k} h_n(y_j) = \sum_{n=0}^{2N} (\bar{D}_k)_{j,n} f(y_n)$$

where

$$(\bar{D}_k)_{j,n} = \frac{d^k h_n(y_j)}{dx^k} .$$

In particular

$$(\bar{D}_1)_{j,n} = \frac{1}{2} \frac{(-1)^{j+n}}{\sin \frac{y_j - y_n}{2}} \qquad j \neq n$$

$$(\bar{D}_1)_{j,j} = 0. \tag{1.15}$$

Moreover, since $h_j(x)$ can be represented as

$$h_j(x) = \frac{2}{2N+1} \sum_{\ell=-N}^{N} e^{i\ell(x-y_j)}$$

we obtain

$$Q_N f(x) = \sum_{\ell=-N}^{N} e^{i\ell x} \frac{2}{2N+1} \sum_{j=0}^{2N} f(y_j) e^{-i\ell y_j} \tag{1.16}$$

so

$$Q_N f(x) = \sum_{\ell=-N}^{N} \bar{a}_\ell e^{i\ell x} \tag{1.17}$$

$$\bar{a}_\ell = \frac{2}{2N+1} \sum_{j=0}^{2N} f(y_j) e^{-i\ell y_j} .$$

With the points z_j defined in (1.1c) the trigonometric interpolant is given by (1.5) with z_j replacing x_j. Equivalently, (1.7) - (1.8) holds with this modification.

Some examples to illustrate the application of the pseudospectral Fourier method follow:

Example 1:

Consider the linear equation

$$Lu \equiv u_{xx} + f(x)u_x + g(x)u = h(x), \tag{1.18}$$

with 2π-periodic boundary conditions. The pseudospectral Fourier equations for the approximation u_N based on the points x_j in (1.1a) are

$$L_N u_N(x_j) \equiv D_2 u_N(x_j) + f(x_j) D_1 u_N(x_j) + g(x_j) u_N(x_j) = h(x_j)$$

$$(j = 0, \cdots, 2N-1) \qquad (1.19)$$

The algebraic system (1.19) may be solved either directly by inverting the $2N \times 2N$ matrix L_N or indirectly by the spectral iteration method explained in Section 8.3.

Example 2:

Consider the nonlinear hyperbolic equation

$$u_t = \frac{1}{2} (u^2)_x \qquad (1.20)$$

with 2π-periodic boundary conditions. The pseudospectral approximation using the points x_j is given explicitly by

$$\frac{\partial u_N}{\partial t} (x_j) = \frac{1}{4} \sum_{\substack{n=0 \\ n \neq j}}^{2N} (-1)^{j+n} \cot \frac{x_j - x_n}{2} u_N^2 (x_n). \qquad (1.21)$$

A suitable time marching technique should be used to solve this system of $2N$ ordinary differential equations in t (see Section 8.2).

2. APPROXIMATION THEORY FOR PERIODIC FUNCTIONS

In this section we discuss various results about the quality of the Fourier approximations described in Section 1. Since we are interested in the application of the pseudospectral method to differential equations it is of interest to determine how good the approximation is, not only for the

solution, but also for its derivatives. The approximation results for the pseudospectral Fourier method turn out to be very similar to Galerkin approximations based on Fourier series (often called spectral approximations), so we review both kinds of results and point out the relation between them here.

If u is a periodic function with p continuous, periodic derivatives, then u can be expanded in a Fourier series of the form

$$u(x) = \sum_{k=-\infty}^{\infty} \hat{a}_k \, e^{ikx}. \tag{2.1}$$

The spectral (Galerkin) approximation to u is given by

$$\hat{P}_N u = \sum_{k=-N}^{N} \hat{a}_k \, e^{ikx} , \tag{2.2}$$

which should be contrasted to the pseudospectral (collocation) approximation (1.7) - (1.8).

For each q, the following quantities are defined:

$$|u|_q^2 = \sum_{k=-\infty}^{\infty} k^{2q} |a_k|^2 \tag{2.3}$$

$$\|u\|_q^2 = \sum_{j=0}^{q} |u|_j^2 . \tag{2.4}$$

The quantity defined in (2.3) is the norm of the qth derivative of u, whereas the norm defined in (2.4) measures the magnitude of u and its first q derivatives.

In theorem (2.1) we quote the principal approximation theory result for the spectral (Galerkin) Fourier method (2.2) (see Canuto and Quarteroni

[1982b] and references cited therein):

THEOREM 2.1 For any $0 \leq q \leq p$, there exists a constant C independent of N and u such that

$$\|u - \hat{P}_N u\|_q \leq C\, N^{q-p}\, |u|_p . \tag{2.5}$$

Theorem 2.1 implies that if u has p derivatives, and the derivatives of $\hat{P}_N u$ (up to qth order) approximate those of u.

At this stage it is interesting to compare the spectral Fourier approximation $\hat{P}_N u$ defined by (2.2) to the pseudospectral Fourier approximation $P_N u$ given by (1.7) - (1.8). From (1.7)

$$a_\ell = \frac{1}{2Nc_\ell} \sum_{j=0}^{2N-1} u(x_j)\, e^{i\ell x_j}. \tag{2.6}$$

Substituting for $u(x_j)$ from (2.1) into (2.6) gives

$$a_\ell = \frac{1}{2Nc_\ell} \sum_{j=0}^{2N-1} e^{-i\ell x_j} \sum_{k=-\infty}^{\infty} \hat{a}_k\, e^{ikx_j}$$

$$= \frac{1}{2Nc_\ell} \sum_{k=-\infty}^{\infty} \hat{a}_k \sum_{j=0}^{2N-1} e^{i(k-\ell)x_j}.$$

Now using the identity

$$\sum_{j=0}^{2N-1} e^{i(k-\ell)x_j} = \begin{cases} 0 & k-\ell \neq 2nN \\ 2N & k-\ell = 2nN \end{cases} \qquad n \text{ integer} \tag{2.7}$$

we obtain

$$a_\ell = \frac{1}{c_\ell} \sum_{n=-\infty}^{\infty} \hat{a}_{\ell+2nN} = \frac{\hat{a}_\ell}{c_\ell} + \frac{1}{c_\ell} \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \hat{a}_{\ell+2nN}. \tag{2.8}$$

Equation (2.8) establishes the relation between $P_N u$ and $\hat{P}_N u$. If u is smooth then $a_k \to 0$ rapidly as $|k| \to \infty$ so the second term on the right side of (2.8) is small.

The main approximation theory result for $P_N u(x)$ is very similar to that for $\hat{P}_N u$, namely:

THEOREM 2.2: Let $p > 1/2$ then for $0 \leq q \leq p$, there exists a constant C independent of N and u such that

$$\|u - P_N u\|_q \leq CN^{q-p} |u|_p , \tag{2.9}$$

(see Canuto and Quarteroni [1982b]).

Unfortunately, the norm defined in (2.4) is not the most natural one for the pseudospectral method. It is more convenient to measure the approximation errors in u and its derivatives at the grid points x_j given by (1.1a). Equivalently, we would like to get a bound on the discrete norm

$$|||u-P_N u|||_q^2 = \sum_{\ell=0}^{q} \frac{1}{2N} \sum_{j=0}^{2N-1} \left[\left(\frac{\partial^\ell u}{\partial x^\ell} - \frac{\partial^\ell P_N u}{\partial x^\ell}\right)(x_j)\right]^2. \tag{2.10}$$

In order to get an estimate for (2.10) we need the following lemma, (Davis and Rabinowitz [1975]).

LEMMA 2.3 Let $f(x)$ be of the form

$$f(x) = \sum_{k=-2N+1}^{2N-1} \hat{f}_k \, e^{ikx}.$$

Then

$$\int_0^{2\ell} f(x)\, dx = \frac{\pi}{2N} \sum_{j=0}^{2N-1} f(x_j).$$

The proof involves a simple application of (2.7). Lemma (2.3) provides the necessary connection between (2.10) and (2.3) to establish the following theorem.

THEOREM 2.4 Let $p > 1/2$, then for $0 \leq q \leq p$, there exists a constant C independent of N and u such that

$$|||u - P_N u|||_q \leq C N^{q-p} |u|_p. \tag{2.11}$$

The error estimates given in (2.5) and (2.11) show the power of the spectral method. The rate of decrease of the error with increasing N only depends on the smoothness of the function u being approximated. However, it is misleading to conclude from (2.5) and (2.11) that if u is not smooth then the approximation $P_N u(x)$ to $u(x)$ is poor. In many applications, one encounters functions u which are piecewise smooth. To illustrate what happens for such u, let us consider a function with a single discontinuity in each period, namely

$$u(x) = x, \quad (|x| \leq \pi)$$

extended periodically in x. The pseudospectral approximation $P_N u$ to u is given by

$$P_N u = \sum_{k=-N}^{N} a_k e^{ikx}$$

where a_k is given by (1.7). In general $\frac{\partial P_N u}{\partial x}$ is a poor approximation to $\partial u/\partial x$ even away from the discontinuity at $x = \pm\pi$. However, if the expansion coefficients a_k are damped as in

$$b_k = a_k \exp\left[-\rho \left(\frac{|k|-k_0}{N-k_0}\right)^4\right] \qquad (|k| \geq k_0), \tag{2.12}$$

then, for suitable choice of ρ and k_0,

$$v(x) = \sum_{k=-N}^{N} b_k e^{ikx}$$

has the property that $\partial v/\partial x$ is a good approximation to $\partial u/\partial x$ away from the points of discontinuities (see Figure 1).

3. STABILITY AND CONVERGENCE OF PSEUDOSPECTRAL FOURIER METHODS

Consider the solution of the time-dependent initial-value problem

$$u_t = Lu \tag{3.1}$$

with initial condition $u(t=0) = u_0$ using the pseudospectral Fourier method. Here L is a linear differential operator with periodic coefficients. The pseudospectral approximate u_N to u satisfies $\frac{\partial u_N}{\partial t} = L_N u_N$, where $u_N(t=0)$ is the trigonometric interpolant of u_0 and L_N is a finite-dimensional approximation to L as explained in Section 1.

The analysis of approximation errors given in Section 2 yields estimates for the truncation error

$$(L - L_N)u \tag{3.2}$$

for differential operators L. It was shown that $(L-L_N)u$ decreases rapidly with N at a rate that depends only on the smoothness of u and the coefficients of the various derivatives appearing in L.

In addition to the consistency properties of a numerical method, the method must be stable to be useful. A scheme is said to be stable if

$$\|u_N(t)\| \leq C\|u_N(0)\| \qquad (0 \leq t \leq T) \tag{3.3}$$

for some appropriate norm. Here C may depend on T, but not on N. The importance of stability derives from the Lax Equivalence Theorem, which implies that if (3.3) is satisfied and $(L-L_N)u \to 0$ as $N \to \infty$ in the same norm as (3.3), then u_N converges to u:

$$\|u-u_N\| \to 0 \qquad (0 \leq t \leq T) \quad \text{as} \quad N \to \infty. \tag{3.4}$$

In other words, stability (3.3) and consistency $\left[(L-L_N)u \to 0\right]$ imply convergence.

In this section, we review some results about the stability and convergence of the pseudospectral Fourier method for hyperbolic and parabolic problems.

Constant Coefficient Wave Equation

Consider the problem

$$u_t = u_x \qquad (0 \leq x \leq 2\pi)$$

$$u(0,t) = u(2\pi,t) \tag{3.5}$$

$$u(x,0) = u_0(x)$$

The pseudospectral Fourier approximation can be written

$$\frac{\partial u_N}{\partial t}(x_k) = \sum_{j=0}^{2N-1} (D_1)_{k,j}\, u_N(x_j) \tag{3.6}$$

where the antisymmetric matrix D_1 is given by (1.10).

The stability of (3.6) can be proven by the energy method. There are two ways of deriving the desired energy estimate. One method is algebraic in nature and uses the structure of the matrix D_1 while the other makes use of the fact that the differential equation is satisfied exactly at the collocation points x_j. These two techniques are extensively used in the theory of spectral methods so we demonstrate them in detail as applied to equations (3.5) - (3.6). In the first case, we multiply (3.6) by $u_N(x_k)$ and sum on k, $(0 \leq k \leq 2N-1)$ to get

$$\sum_{k=0}^{2N-1} u_N(x_k)\, \frac{\partial u_N}{\partial t}(x_k) = \sum_{k=0}^{2N-1} \sum_{j=0}^{2N-1} u_N(x_k)(D_1)_{k,j}\, u_N(x_j)$$

so

$$\frac{1}{2}\frac{d}{dt}\sum_{k=0}^{2N-1} u_N^2(x_k) = \frac{1}{2}\sum_{k=0}^{2N-1}\sum_{j=0}^{2N-1}\left[(D_1)_{k,j} + (D_1)_{j,k}\right]u_N(x_k)u_N(x_j) = 0 \qquad (3.7)$$

since D_1 is an antisymmetric matrix. Equation (3.7) implies energy conservation

$$\sum_{k=0}^{2N-1} u_N^2(x_k,t) = \sum_{k=0}^{2N-1} u_N^2(x_k,0). \qquad (3.8)$$

Therefore the scheme is stable in the sense of (3.3) in the usual L_2 norm.

The second method to establish stability is based on the fact that (3.5) is satisfied at the points x_j

$$\frac{\partial u_N}{\partial t} = \frac{\partial u_N}{\partial x} \quad \text{at} \quad x = x_j = \frac{\pi j}{N} \qquad (j = 0,\cdots,2N-1). \qquad (3.9)$$

Therefore,

$$\frac{1}{2N}\sum_{j=0}^{2N-1} u_N(x_j)\frac{\partial u_N}{\partial t}(x_j) = \frac{1}{2N}\sum_{j=0}^{2N-1} u_N(x_j)\frac{\partial u_N}{\partial x}(x_j). \qquad (3.10)$$

The right side of (3.10) is a trigonometric polynomial of degree $2N-1$, so Lemma 2.3 gives

$$\frac{1}{2N}\sum_{j=0}^{2N-1} u_N(x_j)\frac{\partial u_N}{\partial x}(x_j) = \frac{1}{2\pi}\int_0^{2\pi} u_N(x)\frac{\partial u_N}{\partial x}\,dx = 0,$$

and (3.8) holds.

Similar arguments demonstrate stability for the problem

$$\vec{u}_t = A\,\vec{u}_x \qquad (3.11)$$

where A is a diagonalizable $m \times m$ matrix and $\vec{u}(x,t)$ is a vector with m components. Using the stability result (3.8), it is straightforward to establish an error estimate of the form

$$\|u(t) - u_N(t)\|_0 \leq C(1+N^2)^{\frac{1-q}{2}} \|u_0\|_q \tag{3.12}$$

where the norms are as defined in Section 2.

Variable Coefficient Wave Equation

Consider the problem

$$\begin{aligned} u_t &= a(x)\, u_x \qquad (0 \leq x \leq 2\pi) \\ u(x,0) &= u_0(x) \\ u(0,t) &= u(2\pi,t) \end{aligned} \tag{3.13}$$

with $a(x)$ 2π-periodic. If $a(x) > 0$ for $0 \leq x \leq 2\pi$ then the argument given above shows that

$$\frac{d}{dt} \sum_{j=0}^{2N-1} \frac{u_N^2(x_j)}{a(x_j)} = 0$$

and the same stability and convergence results hold.

However, if $a(x)$ changes sign in $(0,2\pi)$, $u_N(x,t)$ may grow without bound as $t \to \infty$. The following example (Gottlieb, Orszag and Turkel [1981]) illustrates the nature of the instability that may occur. Consider (3.13) with

$$a(x) = \alpha \sin x + \beta \cos x + \gamma. \tag{3.14}$$

For this problem one may derive two different energy estimates. The first one is

$$\|u_N(t)\| \leq e^{\frac{1}{2}(|\alpha|+|\beta|)t}\|u_N(0)\| + 2\sigma_N(e^{\frac{1}{2}(|\alpha| + |\beta|)t} - 1), \tag{3.15}$$

where

$$\|u_N(t)\|^2 = \frac{1}{2N}\sum_{j=0}^{2N-1} u_N^2(x_j,t)$$

and

$$\sigma_N = \sum_{j=0}^{2N-1} (-1)^j u(x_j,0).$$

The second estimate is

$$\|u_N(t)\|_1 \leq e^{\frac{1}{2}(|\alpha|+|\beta|)t} \|u_N(0)\|_1. \tag{3.16}$$

Equations (3.15) and (3.16) prove stability; however the constant C in (3.3) involves $\exp[\frac{1}{2}(|\alpha|+|\beta|T)]$ which grows in time.

The trouble here is the behavior of the solution itself. If $a = 1$, $\beta = \gamma = 0$ in (3.14), then

$$u(x,t) = u_0[2 \tan^{-1}(e^t \tan \tfrac{x}{2})].$$

For large t, the exact solution changes rapidly near $x = 0$ so large values of N are required to resolve this steep gradient. In the literature on numerical methods, this kind of behavior is often referred to as "nonlinear instability" as it often leads to spectacular growth of errors in a nonlinear problem. The problem here can be quite serious in practice but it is not due

to lack of stability in the formal sense, but rather to the lack of spatial resolution. It can be treated either by refining the mesh as the solution develops smaller scales or by treating the region of rapid change as a discontinuity (see below).

Wave Equation with Discontinuity

If the initial condition $u_0(x)$ has a finite number of discontinuities in $[0,2\pi]$ but is otherwise smooth the pseudospectral method is still applicable if some smoothing procedure is used, see Majda, McDonough and Osher [1978] and Mercier [1981]. Typically, one has to modify (1.8) by defining

$$\tilde{u}_N = \sum_{k=-N}^{N} a_k \rho_k e^{ikx} \tag{3.17}$$

where $\rho_k = 1, \ (0 \leq |k| \leq k_0)$

$$\rho_k = e^{-\rho\left(\frac{|k|-k_0}{N-k_0}\right)^4}, \qquad |k| > k_0.$$

It may be shown that, for any q, there is a constant $C_{s,q}$ depending only on $u(t)$, $(0 \leq t \leq T)$ such that

$$\|u(t) - u_N(t)\|_s \leq C_{s,q} N^{-1} \qquad (0 \leq t \leq T). \tag{3.18}$$

Moreover, if the modification (3.17) is applied to the spectral representation of $u_0(x)$,

$$u_0(x) = \sum_{k=-N}^{N} \hat{a}_k \rho_k e^{ikx},$$

then the rate of convergence of u_N to u is arbitrarily fast in any compact region in which $u(x,t)$ is smooth. This shows that the high-order accuracy of the pseudospectral method holds even for nonsmooth problems (Osher (this volume)).

Nonlinear Equations

It is possible to find energy estimates for pseudospectral approximations to nonlinear equations. For example, consider the inviscid Burger's equation (1.20) with initial condition $u(x,0) = u_0(x)$. The pseudospectral approximation (1.21) does not conserve energy but this property can be recovered by rewriting (1.20) as

$$u_t = \frac{1}{3}(u^2)_x + \frac{1}{3}uu_x. \tag{3.19}$$

The pseudospectral approximation to (3.19) is given by

$$\frac{\partial u_N}{\partial t}(x_k) = \frac{1}{3}\sum_{j=0}^{2N-1}(D_1)_{k,j}\,u_N^2(x_j) + \frac{1}{3}\sum_{j=0}^{2N-1}u_N(x_k)(D_1)_{k,j}\,u_N(x_j). \tag{3.20}$$

Multiplying by $u_N(x_k)$ and summing on k gives

$$\frac{1}{2}\frac{d}{dt}\sum_{k=0}^{2N-1}u_N^2(x_k) = 0$$

since D_1 is antisymmetric. Thus, stability is ensured for this pseudospectral scheme.

It is interesting to note that the procedure described above to prove stability may be applied to the Euler equations of gas dynamics. It is known, (see Harten [1983a] and Tadmor [1983]), that the Euler equations can be

expressed in the form

$$H(\vec{v})\vec{v}_t = A(\vec{v})\vec{v}_x \tag{3.21}$$

where $\vec{v}$ is a three-component vector, and $H(\vec{v})$ and $A(\vec{v})$ are 3×3 symmetric matrices. Also, $H(\vec{v})$ is positive definite and H and A satisfy

$$\begin{aligned} H(\vec{v})\vec{v}_t &= [H(\vec{v})\vec{v}]_t \\ A(\vec{v})\vec{v}_x &= [A(\vec{v})\vec{v}]_x. \end{aligned} \tag{3.22}$$

(See Harten [1983a] for the explicit formulas for H and A.) Using (3.22) one rewrite (3.21) as

$$H(\vec{v})\vec{v}_t + [H(\vec{v})\vec{v}]_t = A(\vec{v})\vec{v}_x + [A(\vec{v})\vec{v}]_x. \tag{3.23}$$

For this form of the Euler equations, it follows easily that

$$\frac{d}{dt} \sum_{k=0}^{2N-1} \vec{v}^*(x_k)\, H(\vec{v}(x_k))\vec{v}(x_k) = 0 \tag{3.24}$$

which implies stability in the norm induced by H.

Heat Equation

Consider the problem

$$u_t = u_{xx} \qquad (0 < x < 2\pi)$$

$$u(0,t) = u(2\pi,t) \tag{3.25}$$

$$u(x,0) = u_0(x).$$

The pseudospectral Fourier approximation is

$$\frac{\partial u_N}{\partial t}(x_k) = \sum_{j=0}^{2N-1} (D_2)_{k,j}\, u_N(x_j).$$

Then

$$\frac{\partial u_N}{\partial t} = \frac{\partial^2 u_N}{\partial x^2} \quad \text{at} \quad x = x_k = \frac{\pi k}{N} \qquad (k = 0,\cdots,2N-1) \tag{3.26}$$

so that

$$\frac{\pi}{N} \sum_{k=0}^{2N-1} u_N(x_k) \frac{\partial u_N}{\partial t}(x_k) = \frac{\pi}{N} \sum_{k=0}^{2N-1} u_N(x_k) \frac{\partial^2 u_N(x_k)}{\partial x^2}$$

$$= \int_0^{2\pi} u_N \frac{\partial^2 u_N}{\partial x^2}\, dx = -\int_0^{2\pi} \left(\frac{\partial u_N}{\partial x}\right)^2 dx < 0,$$

proving the stability of this pseudospectral approximation.

4. PSEUDOSPECTRAL CHEBYSHEV METHOD

When a function $f(x)$ is not periodic, a trigonometric interpolation polynomial does not provide a good enough approximation to yield accurate approximations to the derivatives of $f(x)$. It is better to approximate $f(x)$ by polynomials in x. However, it is well known that the Lagrange interpolation polynomial based on equally spaced points does not give a satisfactory approximation to general smooth f. In fact, as the number of collocation points increase, interpolant polynomials typically diverge. This poor behavior of polynomial interpolation can be avoided for smoothly differentiable functions by removing the restriction to equally spaced collocation points. Good results are obtained by relating the collocation points to the structure of classical orthogonal polynomials, like Chebyshev or Legendre polynomials.

In the most common pseudospectral Chebyshev method, the interpolation points in the interval $(-1,1)$ are chosen to be the extrema

$$x_j = \cos \frac{\pi j}{N} \qquad (j = 0,\cdots,N) \tag{4.1}$$

of the Nth order Chebyshev polynomials $T_N(x)$. Here the Chebyshev polynomial of degree n is defined by

$$T_n(x) = \cos(n \cos^{-1} x). \tag{4.2}$$

It follows that

$$T_n(x_j) = \cos \frac{\pi j n}{N} \tag{4.3}$$

which indicates a close relation between the pseudospectral Chebyshev and the

pseudospectral Fourier method. In order to construct the interpolant of $f(x)$ at the point x

$$g_j(x) = \frac{(1-x^2)T_N'(x)(-1)^{j+1}}{\bar{c}_j N^2 (x-x_j)} \qquad (j = 0,\cdots,N) \tag{4.4}$$

with $\bar{c}_0 = \bar{c}_N = 2$, $\bar{c}_j = 1$, $(1 \leq j \leq N-1)$. It is readily verified that

$$g_j(x_k) = \delta_{jk}.$$

The Nth degree interpolation polynomial, $P_N f(x)$, to $f(x)$ is given by

$$P_N f(x) = \sum_{j=0}^{N} f(x_j)\, g_j(x). \tag{4.5}$$

A different way of representing $P_N f(x)$ is to use the identity

$$\sum_{n=0}^{N} \frac{T_n(x_j)T_n(x)}{\bar{c}_n} = \frac{(1-x^2)T_N'(x)}{2N(x-x_j)} (-1)^{j+1}$$

giving

$$\sum_{j=0}^{N} f(x_j)g_j(x) = \frac{2}{N} \sum_{j=0}^{N} \frac{f(x_j)}{\bar{c}_j} \sum_{n=0}^{N} \frac{T_n(x_j)T_n(x)}{\bar{c}_n}$$

$$= \frac{2}{N} \sum_{n=0}^{N} T_n(x) \frac{1}{\bar{c}_n} \sum_{j=0}^{N} \frac{f(x_j)T_n(x_j)}{\bar{c}_j}.$$

Thus,

$$P_N f(x) = \sum_{n=0}^{N} a_n T_n(x) \tag{4.6}$$

where

$$a_n = \frac{2}{N} \frac{1}{\bar{c}_n} \sum_{j=0}^{N} \frac{f(x_j)T_n(x_j)}{\bar{c}_j}. \tag{4.7}$$

It should be noted that the coefficients a_n in (4.7) can be evaluated using the FFT. In fact, using (4.3) in (4.7) gives

$$a_n = \frac{2}{N} \frac{1}{\bar{c}_n} \sum_{j=0}^{N} \frac{f(x_j)}{\bar{c}_j} \cos \frac{\pi j n}{N} . \tag{4.8}$$

The second step in getting a pseudospectral approximation is to express the derivations of $P_N f$ in terms of $f(x)$ at the collocation points x_j. This can be done by differentiating either (4.5) or (4.6). With (4.5) we obtain

$$\frac{d^p P_N f(x)}{dx^p} = \sum_{j=0}^{N} f(x_j) \frac{d^p}{dx^p} g_j(x) \tag{4.9}$$

so that

$$\frac{d^p P_N f(x_k)}{dx^p} = \sum_{j=0}^{N} f(x_j)(D_p)_{k,j} \tag{4.10}$$

where

$$(D_p)_{k,j} = \frac{d^p}{dx^p} g_j(x) \Big|_{x=x_k} . \tag{4.11}$$

For example

$$(D_1)_{k,j} = \frac{\bar{c}_k}{\bar{c}_j} \frac{(-1)^{j+k}}{x_k - x_j} \qquad (k \neq j) \tag{4.12}$$

$$(D_1)_{j,j} = \frac{x_j}{2(1-x_j^2)} , \quad (D_1)_{00} = \frac{2N^2 + 1}{6} = - (D_1)_{NN}$$

and

$$D_p = (D_1)^p . \tag{4.13}$$

It should be noted from the explicit formula (4.12) that the matrix D_1 is not antisymmetric; also D_2 is not symmetric. These facts introduce both theoretical and practical difficulties in the pseudospectral Chebyshev method.

A different way to obtain an expression for the derivative of $P_N f$ is to differentiate (4.6) to get

$$\frac{d^p}{dx^p} P_N f = \sum_{n=0}^{N} a_n T_n^{(p)}(x),$$

where the coefficients a_n are given by (4.7). For example,

$$\frac{d P_N f}{dx} = \sum_{n=0}^{N} a_n T_n'(x) = \sum_{n=0}^{N} b_n T_n(x) \qquad (4.15)$$

where

$$b_N = 0, \quad b_{N-1} = 2N a_N$$

and

$$\bar{c}_n b_n = b_{n+2} + 2(n+1)a_{n+1} \qquad (0 \leq n \leq N-2). \qquad (4.16)$$

In evaluating the first derivative at the collocation points x_j the FFT is used to evaluate a_n by (4.8) and then

$$\frac{d}{dx} P_N f(x_j) = \sum_{n=0}^{N} b_n \cos \frac{\pi n j}{N}$$

More generally

$$\frac{d^p (P_N f)}{dx^p} = \sum_{n=0}^{N} b_n^{(p)} T_n(x)$$

where $b_n^{(0)} = a_n$, $0 \leq n \leq N$, $b_n^{(1)} \equiv b_n$, and

$$\bar{c}_n \, b_n^{(p)} = b_{n+2}^{(p)} + 2(n+1)b_{n+1}^{(p-1)},$$

with

$$b_N^{(p)} = 0, b_{N-1}^{(p)} = 2Nb_N^{(p-1)}. \tag{4.17}$$

The set of points x_j defined in (4.1) is not the only set used with pseudospectral Chebyshev approximations. For hyperbolic problems, a convenient alternative set of collocation points is

$$y_j = \cos \frac{\pi j}{N+1} \qquad (j = 0, \cdots, N). \tag{4.18}$$

The interpolation polynomial at the points y_j is of degree N and is given by

$$Q_N f = \sum_{j=0}^{N} f(y_j) h_j(x)$$

where

$$h_j(x) = \frac{(-1)^{j+1}}{\bar{c}_j (N+1)^2} \frac{(1-x)(1+y_j) T'_{N+1}(x)}{(x-y_j)}. \tag{4.19}$$

Upon differentiation, we obtain

$$\frac{d(Q_N f)}{dx}(y_k) = \sum_{j=0}^{N} (\hat{D}_1)_{kj} f(y_j) \qquad (k = 0, \cdots, N) \tag{4.20}$$

where

$$(\hat{D}_1)_{k,j} = \frac{1+y_j}{1+y_k} (D_1)_{k,j}$$

and D_1 is given by (4.12).

It is clear from (4.4) and (4.19) that, for every function $f(x)$, $(-1 \leq x \leq 1)$,

$$(1 + x)\, Q_N f(x) = P_{N+1}[(1+x) f(x)].$$

Moreover, if $Q_N f(x)$ is expanded in terms of Chebyshev polynomials,

$$Q_N f = \sum_{n=0}^{N} \bar{a}_n T_n(x), \tag{4.21}$$

there is a simple relation between $\{\bar{a}_n\}$ and $\{a_n\}$ defined in (4.7) with $N \leftarrow N + 1$. In fact,

$$Q_N f = Q_N(P_{N+1} f) = P_{N+1} f + \frac{a_{N+1}}{N+1} (1-x) T'_{N+1}(x) \tag{4.22}$$

so, recalling the derivation of (4.6) - (4.7),

$$\bar{a}_n = a_n + 2(-1)^{n+N+1} a_{N+1} \qquad (1 \leq n \leq N). \tag{4.23}$$

Equation (4.23) shows that FFT techniques can also be used with the set of points y_j.

The other two sets of points that are sometimes used are

$$z_j^{(1)} = \cos \frac{2\pi j}{2N+1} \qquad (j = 0, \cdots, N) \tag{4.24}$$

and

$$z_j^{(2)} = \cos \frac{\pi(2j+1)}{2N+1} \qquad (j = 0, \cdots, N). \tag{4.25}$$

5. APPROXIMATION THEORY OF THE PSEUDOSPECTRAL CHEBYSHEV METHOD

In order to measure the approximation error between f and $P_N f$ defined in Section 4, we introduce the norms

$$\|f\|^2 = \int_{-1}^{1} \frac{f^2(x)}{\sqrt{1-x^2}}\, dx \tag{5.1}$$

$$\|f\|_q^2 = \left[\|f\|^2 + \|\frac{\partial f}{\partial x}\|^2 + \cdots + \|\frac{\partial^q f}{\partial x^q}\|^2\right]. \tag{5.2}$$

These norms are useful since we are interested in applying the pseudospectral method to the solution of differential equations and hence we need to measure the error between the derivatives of the solution and those of the approximation.

The main approximation result is summarized in the following theorem.

THEOREM 5.1 Let $f(x)$ be a function with s continuous derivatives and let $P_N f$ be defined as in Section 4. Then, there is a constant C independent of $f(x)$ and N such that

$$\|f-P_N f\|_q \leq C\, N^{2q-s}\, \|f\|_s, \quad (0 \leq q \leq \tfrac{1}{2} s). \tag{5.3}$$

The difference between (5.3) and (2.8) should be noted. Each derivative on the left side of (5.3) introduces a new factor of N^2 in the error estimate rather than the factor N appearing in (2.8).

As before, the norms defined in (5.1) and (5.2) should be modified in order to reflect the errors at the collocation points. To do this, we use the following two lemmas:

LEMMA 5.2 (see Rivlin [1974]): Let $g(x)$ be a polynomial of degree $2N - 1$ and let $x_j = \cos \pi j/N$, $(j = 0, \cdots, N)$. Then,

$$\frac{\pi}{N} \sum_{j=0}^{N} \frac{g(x_j)}{\bar{c}_j} = \int_{-1}^{1} \frac{g(x)}{\sqrt{1 - x^2}}\, dx, \tag{5.4}$$

where $\bar{c}_0 = \bar{c}_N = 2$, $\bar{c}_j = 1$, $(1 \leq j \leq N-1)$.

LEMMA 5.3 Let $f(x)$ be a polynomial of degree N then

$$\int_{-1}^{1} \frac{f^2(x)}{\sqrt{1 - x^2}}\, dx \leq \frac{\pi}{N} \sum_{j=0}^{N} \frac{f^2(x_j)}{\bar{c}_j} \leq 2 \int_{-1}^{1} \frac{f^2(x)}{\sqrt{1 - x^2}}\, dx. \tag{5.5}$$

This lemma is proven using Lemma 5.2 after representing $f^2(x)$ as a mixture of $T_{2N}(x)$ plus a polynomial of degree $2N - 1$. Using Lemma 5.3 we get the following error estimate.

THEOREM 5.4 Let

$$h(x) = f(x) - P_N f(x).$$

Then

$$\frac{\pi}{N} \sum_{\ell=0}^{q} \sum_{j=0}^{N} \left(\frac{\partial^\ell h(x_j)}{\partial x^\ell}\right)^2 \leq C\, N^{2q-s}\, \|f\|_s, \tag{5.6}$$

where C is independent of f and N.

When $f(x)$ is discontinuous at one (or a finite number) of points, we can still obtain a good approximation for the derivative far away from the discontinuity. In order to do so, we modify the expression for $P_N f$ as in

$$\tilde{P}_N f = \sum_{n=0}^{N} a_n \rho_n T_n(x), \tag{5.7}$$

where

$$\rho_n = 1 \qquad (n \leq n_0)$$

$$\rho_n = \exp\left[-\rho\left(\frac{n-n_0}{N-n_0}\right)^4\right] \qquad (n_0 < n \leq N). \tag{5.8}$$

In Figure 2 we plot the derivative of a step function with and without the smoothing described in (5.7) - (5.8).

6. STABILITY AND CONVERGENCE OF PSEUDOSPECTRAL CHEBYSHEV METHODS

In this section we review some results concerning the stability and convergence of the pseudospectral Chebyshev method. The most common way to prove stability is to use energy estimates similar to those used to demonstrate the well-posedness of the differential equation. This approach is not systematic; one has to guess a suitable norm in which the energy is bounded. An alternative approach is to solve explicitly the equation for the error and then to verify stability. This approach to the analysis of spectral methods was introduced by Dubiner in unpublished work that is reviewed in the Appendix.

Results for Parabolic Equations

Consider the equation

$$\frac{\partial u}{\partial t} = a(x)\,\frac{\partial^2 u}{\partial x^2} \qquad (|x| < 1) \tag{6.1a}$$

$$u(-1,t) = g(t), \qquad u(1,t) = h(t) \tag{6.1b}$$

$$u(x,0) = u_0(x), \qquad a(x) \geq a_0 > 0. \tag{6.1c}$$

The pseudospectral Chebyshev approximation $u(x,t)$ is an Nth degree polynomial in x that satisfies

$$\frac{\partial u_N}{\partial x} = a(x)\,\frac{\partial^2 u_N}{\partial x^2} \qquad \left(x = x_j \equiv \cos\frac{\pi j}{N}\,,\ \ 0 < j < N\right) \tag{6.2}$$

$$u_N(-1,t) = g(t), \qquad u_N(1,t) = h(t).$$

The stability of this method is easily demonstrated by an energy argument. In fact (6.2) gives (with $g \equiv h \equiv 0$)

$$\frac{\pi}{N} \sum_{j=0}^{N} \frac{u_N(x_j,t)}{a(x_j)}\,\frac{\partial u_N}{\partial t}(x_j,t) = \frac{\pi}{N} \sum_{j=0}^{N} u_N(x_j)\,\frac{\partial^2 u_N}{\partial x^2}(x_j). \tag{6.3}$$

Then, Lemma (5.2) implies that

$$\frac{\pi}{2N}\,\frac{d}{dt} \sum_{j=0}^{B} \frac{u_N^2(x_j,t)}{a(x_j)} = \int_{-1}^{1} \frac{\partial^2 u_N}{\partial x^2}\,\frac{u_N\,dx}{\sqrt{1-x^2}}\,. \tag{6.4}$$

The right side of (6.4) is non-positive (see Gottlieb and Orszag [1977], p. 82) so that

$$\sum_{j=0}^{N} \frac{u_N^2(x_j,t)}{a(x_j)} \leq \sum_{j=0}^{N} \frac{u_N^2(x_j,0)}{a(x_j)} . \tag{6.5}$$

The stability of the scheme (6.2) gives the following error estimate:

Theorem 6.1 (Canuto and Quarteroni [1981]): Let $\sigma > 1/2$, $s > \sigma + 2$, $0 < t < T$, and suppose that $u(x,t)$ has s spatial derivatives, then there is a constant C independent of u and N such that

$$\frac{\pi}{N} \sum_{j=0}^{N} \frac{1}{\bar{c}_j} \left| u_N(x_j,t) - u(x_j,t) \right|^2 \leq CN^{2\sigma+4-s}.$$

A similar proof may be applied to (6.1) when the boundary conditions are of Neumann type, i.e., $u_x(\pm 1,t)$ are given. For the Neumann problem we get the following stability estimate.

THEOREM 6.2: Let $u_N(x,t)$ be the pseudospectral Chebyshev approximation to the solution u of (6.1) (with $a(x) = 1$) and boundary conditions $u_x(\pm 1,t) = 0$. Suppose that u_N has a Chebyshev expansion of the form

$$u_N(x,t) = \sum_{n=0}^{N-1} w_k \, T_k(x) + w_N(t) T_N(x).$$

Then,

$$\frac{d}{dt} \left[\int_{-1}^{1} \sqrt{1 - x^2} \left(\frac{\partial u_N}{\partial x} (x,t) \right)^2 dx + N^2 \, w_N^2(t) \right] \leq 0. \tag{6.6}$$

Note that the norm used in (6.6) differs from the one used in (6.5).

If $a(x) \equiv 1$ and $g(t) = h(t) = 0$) then it is possible to gain more information about the pseudospectral Chebyshev approximation to (6.1) by

explicitly studying the eigenvectors and eigenvalues of the finite-dimensional pseudospectral approximation. Since $u_N(x,t)$ is a polynomial of degree N in x so is $E_N(x,t)$ defined by

$$E_N(x,t) = \left(\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}\right)u_N.$$

Moreover, since $E_N(x,t)$ vanishes at the points x_j (which are the roots of T_N'), it follows that

$$E_N(x,t) = \left(\hat{A}(t) + \hat{B}(t)x\right) T_N'(x)$$

for appropriate functions $\hat{A}(t)$, $\hat{B}(t)$. Assume that

$$u_N(x,t) = e^{\lambda t}\, v_N(x). \tag{6.7}$$

Then $\hat{A}(t) = Ae^{\lambda t}$, $B(t) = \hat{B}e^{\lambda t}$ so $v_N(x)$ satisfies

$$\lambda v_N(x_j) - \frac{\partial^2 v_N(x_j)}{\partial x^2} = (A + Bx)T_N'. \tag{6.8}$$

Therefore

$$v_N(x) = A\,\phi_N(x,\lambda) + B\chi_N(x,\lambda) \tag{6.9}$$

where

$$\phi_N(x,\lambda) = \sum_{k=0}^{\infty} \lambda^{-k-1} \frac{\partial^{2k+1}}{\partial x^{2k+1}} T_N(x) \tag{6.10a}$$

and

$$\chi_N(x,\lambda) = \sum_{k=0}^{\infty} \lambda^{-k-1} \frac{\partial^{2k}}{\partial x^{2k}} \left(x \frac{\partial T_N}{\partial x}\right). \tag{6.10b}$$

We assume for simplicity that N is even and therefore $\phi_N(x,\lambda)$ is an odd function of x and $\chi_N(x,\lambda)$ is an even function of x. For the Dirichlet problem with homogeneous boundary conditions the eigenvalues λ are obtained by solving

$$\phi_N(1,\lambda)\ \chi_N(1,\lambda) = 0. \tag{6.11}$$

Upon setting $\mu = \frac{1}{\lambda}$, it follows that ϕ_N is a polynomial of degree $\frac{N}{2} - 1$ in μ while χ_N is a polynomial of degree $\frac{N}{2}$ in μ. It has been shown (Gottlieb and Lustman [1982]) that the roots of $\phi_N(1, \frac{1}{\mu})$ are real, negative, and distinct as are those of $\chi_N(1, \frac{1}{\mu})$. Therefore, (6.11) yields $N - 1$ real, negative, and distinct eigenvalues which is the required number of roots since there are $N - 1$ interior points in the scheme.

In conclusion we have now explicitly $N - 1$ eigenfunctions

$$\phi_N(x,\lambda_1),\cdots,\phi_N(x,\lambda_{\frac{N}{2}-1}),\chi_N(x,\nu_1),\cdots,\chi_N(x,\nu_{\frac{N}{2}}), \tag{6.12}$$

where $\lambda_1,\cdots,\lambda_{\frac{N}{2}-1}$ are the roots of $\phi_N(1,\lambda)$ and $\nu_1,\cdots,\nu_{\frac{N}{2}}$ are those of $\chi_N(1,\lambda)$.

Consider now the more general case of boundary conditions

$$\begin{aligned} \alpha u(1) + \beta u_x(1) &= 0 \\ \gamma u(-1) + \delta u_x(-1) &= 0. \end{aligned} \tag{6.13}$$

There are as yet no stability proofs for the pseudospectral Chebyshev method for (6.1) with (6.13). The difficulty in finding an energy estimate is that the norm used for Dirichlet boundary conditions is different from that used

for Neumann boundary conditions. However, it is still possible to find the eigenvalues and eigenvectors for this problem. As a matter of fact the eigenvalues are given by the roots η_i of the polynomial equation

$$\left[\alpha\phi_N(1,\eta) + \beta \frac{\partial \phi_N}{\partial x}(1,\eta)\right]\left[\gamma\chi_N(1,\eta) - \delta \frac{\partial \chi_N}{\partial x}(1,\eta)\right]$$

$$+ \left[\alpha\chi_N(1,\eta) + \beta \frac{\partial \chi_N}{\partial x}(1,\eta)\right]\left[\gamma\phi_N(1,\eta) - \delta \frac{\partial \phi_N}{\partial x}(1,\eta)\right] = 0. \qquad (6.14)$$

It may be shown that the roots $\eta_i (i = 1,\cdots,N-1)$ of (6.14) are real, negative, and distinct if α and β are of the same sign.

The results for the eigenvalue analysis indicate that, for fixed number of mesh points N, the pseudospectral approximation converges to a steady state as $t \to +\infty$ as does the analytic solution to (6.1). The analysis does not prove convergence of u_N to u as N increases. However, it is important to know the structure of the eigenvalues and eigenvectors to fully understand the behavior of the approximation.

Results for Scalar Hyperbolic Problems

Let us start by considering the scalar equation

$$\begin{aligned} u_t &= u_x \qquad (|x| < 1) \\ u(x,0) &= f(x) \\ u(1,t) &= g(t). \end{aligned} \qquad (6.15)$$

For this simple equation all the methods described in Section 4 are applicable. We shall review here the theory for the pseudospectral approximation based on the points y_j defined in (4.18). The use of other points will be discussed later.

Let u_N be the pseudospectral Chebyshev approximation to u, then u_N satisfies

$$\frac{\partial u_N}{\partial t} = \frac{\partial u_N}{\partial x} \qquad (x = y_j,\ j = 1,\cdots,N)$$

$$u_N(1,t) = u_N(y_0,t) = g(t) \tag{6.16}$$

$$u_N(x,0) = P_N f(x).$$

Then the following inequality holds (Gottlieb [1981])

$$\frac{\pi}{N}\frac{d}{dt}\sum_{j=1}^{N}(1+y_j)u_N^2(y_j,t) + \frac{\pi}{8N}u_N^2(-1,t) \leq \frac{\pi N}{6}g^2(t). \tag{6.17}$$

which gives the following error estimate:

$$\frac{\pi}{N}\sum_{j=0}^{N}(1+y_j)\left[u(y_j,t) - u_N(y_j,t)\right]^2 \leq CN^{2(1+\sigma)-s} \tag{6.18}$$

where $\sigma > 1/2$ and $s > 2(1+\sigma)$, s is the number of derivatives possessed by the initial conditions and the constant C is independent of u and N. Similar results hold for the points $z_j^{(1)}$, $z_j^{(2)}$ defined in (4.24). Unfortunately, there is still no estimate of the form (6.17) and (6.18) for the set of points x_j defined in (4.1) which is the set most commonly used in applications.

If the differential equation is of the slightly more general form

$$u_t = c(x)\,u_x \qquad (|x| < 1),$$

where $c(x)$ does not change sign in the domain, the above results still hold. The case in which $c(x)$ changes sign introduces some difficulty. The following examples illustrate the kinds of problems that may arise. Consider the two equations

$$\begin{aligned} u_t &= xu_x \qquad (|x| < 1) \\ u(x,0) &= f(x) \\ u(1,t) &= f(e^t), \quad u(-1,t) = f(-e^t), \end{aligned} \tag{6.19}$$

whose analytic solution is $u(x,t) = f(xe^t)$, and

$$\begin{aligned} u_t &= -xu_x \qquad (|x| < 1) \\ u(x,0) &= f(x), \end{aligned} \tag{6.20}$$

with solution $u = f(xe^{-t})$. The pseudospectral Chebyshev approximation to both problems has been shown to be stable (Gottlieb [1981]). However, there is a noticable difference between the behavior of the error for (6.19) and (6.20). For (6.19), there is significant loss of accuracy as t increases. This is due to the fact that the gradient of the solution grows with time as e^t and, therefore, with fixed number of grid points, the numerical approximation can not resolve the steep gradients. This phenomenon does not occur when (6.20) is solved.

When the differential equation being solved is nonlinear, behavior similar to that encountered for (6.19) may occur in the numerical approximation, except now the solution may diverge explosively in a finite time rather than having just gradual loss of accuracy in time. Smoothing, done by cutting high modes, should be applied in these cases to avoid such "nonlinear instabilities".

Results for Systems of Hyperbolic Equations

Consider the symmetric 2×2 system

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1/2 & 1 \\ 1 & 1/2 \end{pmatrix} \frac{\partial}{\partial x}\begin{pmatrix} u \\ v \end{pmatrix} \tag{6.21}$$

$$u(-1) = f(t), \quad u(1) = g(t)$$

$$\begin{pmatrix} u \\ v \end{pmatrix}_{x=0} = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}.$$

For such a non-diagonal system, the points $z_j^{(1)}$, $z_j^{(2)}$ are not easily applicable. Therefore, we shall discuss the pseudospectral method for the set of collocation points $x_j = \cos \frac{\pi j}{N}$, $(j = 0, \cdots, N)$. (Similar results hold for the points y_j.) Assume that u and v are known at some time t_1 and that we would like to advance to the time level t_2. First, we get the value of $u_x(x,t_1)$ and $v_x(x,t_1)$ by the pseudospectral procedure described in Section 4. Then we multiply by the matrix $\begin{pmatrix} 1 & 1/2 \\ 1/2 & 1 \end{pmatrix}$ and advance in time to t_2. This algorithm gives values for u and v at the time t_2 at each of the collocation points x_j, which we shall denote by $u^c(x_j,t_2)$ and $v^c(x_j,t_2)$. Then we set

$$\begin{aligned} u(x_j,t_2) &= u^c(x_j,t_2) \qquad (j = 1, \cdots, N-1) \\ v(x_j,t_2) &= v^c(x_j,t_2) \qquad (j = 0, \cdots, N) \end{aligned} \tag{6.22}$$

$$u(-1,t_2) = f(t_2), \quad u(-1,t_2) = g(t_2).$$

It turns out that the pseudospectral method just described is unstable, although the differential equation is well posed. Instead of (6.22), improved boundary conditions may be shown to lead to a stable scheme. The form of these conditions is suggested by using characteristic variables which are, in this example, $u + v$ on the characteristic $dx/dt = -3/2$ and $u - v$ on the incoming characteristic should be specified at $x = -1$ whereas $u + v$ at $x = -1$ is carried out on an outgoing characteristic and should be determined by the time-marching scheme. Similarly $u + v$ should be given at $x = 1$ while $u - v$ at $x = -1$ should be given by the time-marching scheme. The procedure described by (6.22) is unstable because it uses the numerical scheme (at $x = -1$) to find v rather than $u + v$. The scheme is stabilized by requiring that $u + v$ at $x = -1$ and $u - v$ at $x = 1$ have the values computed by the time-marching scheme from the previous time level, even aftr imposition of the boundary conditions on $u(\pm 1, t_2)$. Thus (6.22) is replaced by

$$
\begin{aligned}
&u(x_j,t_2) = u^c(x_j,t_2) && (j = 1,\cdots,N-1)\\
&v(x_j,t_2) = v^c(x_j,t_2) && (j = 1,\cdots,N-1)\\
&u(x_0,t_2) = f(t_2),\quad u(x_N,t_2) = g(t_2) && \qquad (6.23)\\
&u(x_0,t_2) - v(x_0,t_2) = u^c(x_0,t_2) - v^c(x_0,t_2)\\
&u(x_N,t_2) + v(x_N,t_2) = u^c(x_N,t_2) + v^c(x_N,t_2).
\end{aligned}
$$

In general when a hyperbolic system of equations is solved one should use the time-marching scheme to determine the boundary values of the outgoing characteristic variables. This procedure yields stable results. Applications to multi-dimensional problems are given by Gottlieb, Lustman & Streett, (this volume).

Eigenvalues and Eigenvectors for Hyperbolic Equations

As in the case of parabolic equations it is possible to find explicitly the eigenvectors and the characteristic equations for the Chebyshev approximations to (6.16). Let u_N denote the approximation to the solution of (6.16) based on the points x_j and let v_N denote the approximations based on the points y_j. Then u_N and v_N satisfy exactly

$$\begin{aligned} \frac{\partial u_N}{\partial t} &= \frac{\partial u_N}{\partial x} + \tau \frac{(1+x)T_N'}{2N^2} \\ \frac{\partial v_N}{\partial t} &= \frac{\partial v_N}{\partial x} + \bar{\tau} \frac{T_{N+1}'}{N^2} \end{aligned} \tag{6.24}$$

for suitable τ, $\bar{\tau}$. Assuming that $u_N = e^{\lambda t}\hat{u}_N$, $v_N = e^{\mu t}\hat{v}_N$ and substituting into (6.24), one obtains

$$\begin{aligned} \frac{\partial \hat{u}_N}{\partial x} &= \lambda u_N + \alpha \frac{(1+x)T_N'}{2N^2} \\ \frac{\partial \hat{v}_N}{\partial x} &= \mu \hat{v}_N + \beta \frac{T_{N+1}'}{N^2}, \end{aligned} \tag{6.25}$$

for suitable α, β. Therefore

$$\begin{aligned} \hat{u}_N(x) &= \sum_{k=0}^{\infty} \lambda^{-k-1} \frac{d^k}{dx^k} \frac{(1+x)T_N'}{2N^2} \\ \hat{v}_N(x) &= \sum_{k=0} \mu^{-k-1} \frac{d^{k+1}}{dx^{k+1}} \frac{T_{N+1}}{N^2}, \end{aligned} \tag{6.26}$$

where λ and μ are determined by the eigenvalue conditions

$$\hat{u}_N(1) = 0$$

$$\hat{v}_N(1) = 0.$$

All the eigenvalues satisfy $\text{Re } \lambda < 0$, $\text{Re } \mu < 0$.

7. OTHER POLYNOMIAL EXPANSIONS

Although most of the actual computations with spectral methods involve expansion with trigonometric function and Chebyshev polynomials, there are other basis functions that are currently being used. Here we briefly review some of those methods.

Legendre Polynomials

An attractive alternative to Chebyshev polynomial expansions is Legendre polynomial expansions. It suffices to explain how to construct a pseudospectral Legendre polynomial approximation to a derivative.

Let $x_0 = -1$, $x_N = 1$, and let $x_i, (i = 1, \cdots, N-1)$ be the roots of $q_N'(x)$, where $q_N(x)$ is the Legendre polynomial of degree N. Given the values of any function $f(x)$ at the points x_j $(j = 0, \cdots, N)$, we construct the interpolating polynomials

$$P_N f = \sum_{j=0}^{N} f(x_j)\, g_j(x), \tag{7.1}$$

where

$$g_j(x) = -\frac{1}{\alpha_N\, q_N(x_j)} \frac{(1-x^2)q_N'(x)}{x - x_j}$$

with

$$\alpha_N = N(N+1).$$

Therefore

$$\frac{d^\ell}{dx^\ell} P_N f\Big|_{x=x_k} = \sum_{j=0}^{N} f(x_j) \frac{\partial^\ell g_j(x_k)}{\partial x^\ell} = \sum_{j=0}^{N} (D_\ell)_{kj} f(x_j). \qquad (7.2)$$

For example

$$(D_1)_{kj} = \frac{q_N(x_k)}{q_N(x_j)} \frac{1}{x_k - x_j} \qquad (k \neq j)$$

$$(D_1)_{00} = \frac{1}{4} \alpha_N = - (D_1)_{NN} \qquad (7.3)$$

$$(D_1)_{kk} = 0 \qquad (k \neq 0,\ k \neq N).$$

The difference between the Chebyshev and Legendre methods is evident here. The matrix D_1 for Legendre polynomials is nearly antisymmetric, in contrast to the Chebyshev matrix given in (4.12).

By the same method, we obtain

$$(D_2)_{kj} = -2 \frac{q_N(x_k)}{q_N(x_j)} \frac{1}{(x_k - x_j)^2} \qquad 1 \leq k, j \leq N-1,\ k \neq j$$

$$(D_2)_{jj} = - \frac{1}{3} \frac{N}{1 - x_j^2} \qquad 1 \leq j \leq N-1. \qquad (7.4)$$

This shows that $D_2 = \Lambda S \Lambda^{-1}$, where Λ is a diagonal matrix and S is symmetric.

The following result indicates that the accuracy of Legendre approximation is comparable with the accuracy of Chebyshev approximations:

THEOREM 7.1: Let $f(x)$ have σ smooth derivatives for $|x| \leq 1$, and define $\|f\|^2 = \sum_{\ell=0}^{\sigma} \int_{-1}^{1} \left(\frac{d^\ell f}{dx^\ell}\right)^2 dx$. Then there is a constant C independent of $f(x)$ and N such that

$$\sum_{\ell=0}^{\mu} \left[\sum_{j=0}^{N} \left(\frac{d^\ell f}{dx^\ell}(x_j) - \frac{d^\ell P_N f(x_j)}{dx^\ell}\right)^2 \right]^{1/2} \leq CN^{2\mu-\sigma} \|f\|_\sigma \tag{7.5}$$

for $\mu < \frac{1}{2}\sigma$.

Stability results are much easier to obtain here than with Chebyshev approximation. For example, consider the pseudospectral Legendre method for the approximation of

$$\begin{aligned} u_t &= u_x \qquad (|x| < 1). \\ u(1,t) &= 0 \end{aligned} \tag{7.6}$$

From (7.3) it follows that

$$\frac{1}{2}\frac{d}{dt} \sum_{k=0}^{N} \frac{1}{[q_N(x_k)]^2} u_N^2(x_k) = \sum_{k=0}^{N} \sum_{j=0}^{N} \frac{1}{[q_N(x_k)]^2} (D_1)_{kj} u_N(x_j) u_N(x_k)$$

$$= \frac{1}{2} \sum_{k=0}^{N} \sum_{j=0}^{N} \frac{(D_1)_{kj}}{[q_N(x_k)]^2} + \frac{(D_1)_{jk}}{[q_N(x_j)]^2} u_N(x_j) u_N(x_k) \tag{7.7}$$

$$= -\frac{1}{2} \alpha_N \frac{u^2(x_N)}{q_N^2(x_N)} < 0$$

showing stability.

A similar proof holds for parabolic equations.

Jacobi Polynomials

An interesting use of a different set of expansion functions was suggested by Wray & Leonard [1982] for the case of three-dimensional flow in a pipe. The velocity vector $\vec{u}$ is expanded

$$\vec{u}(r,\theta,x,t) = \sum_{n,k,\ell} a_{m,k,\pi}(t)\ \vec{\chi}_{m,k,\ell}(r)\ \exp(ikx + i\ell\theta). \qquad (7.8)$$

The vector $\vec{\chi}(r)$ is expressed in terms of q_n^{ℓ} where

$$q_n^{\ell} = r^{|\ell|}(1-r^2)^2\ g_n^{|\ell|}\ (r^2),$$

where $g_n^{\ell}(y)$ is the shifted Jacobi polynomial

$$g_n^{\ell}(y) = P_n^{(0,\ell)}(2y-1).$$

With this choice of basis function, one gets the correct behavior of $\vec{u}$ as $r \to 0$. Moreover, since $q_n^{(\ell)}$ satisfy the orthogonality condition

$$\int_0^1 y\ q_m^{(\ell)}(y)\ q_n^{(\ell)}(y)dy = c_m^{\ell}\ \delta_{m,n}\ ,$$

one gets simple expressions for the derivatives. For example, one can show that

$$\nabla^2[q_n^{\ell}(r)\exp(i\ell\theta)] = r^{\ell}[b_n^{\ell}\ q_{n-1}^{(\ell)} + c_n^{\ell}\ q_n^{(\ell)} + d_n^{\ell}\ q_{n+1}^{(\ell)}]\exp(i\ell\theta),$$

for certain constants b_n^{ℓ}, c_n^{ℓ}, d_n^{ℓ} .

8. TIME DISCRETIZATION AND ITERATIVE METHODS

8.1 Time Discretization

One of the major difficulties in the application of spectral methods to flow problems is time marching methods. We may divide flow problems into three categories. First, we have problems in which we are interested only in steady state solutions. These problems require a time marching technique which may be inaccurate, but should converge fast to the steady state solution. Discussion of these methods will be given in Subsection 8.3. The second class of problems are those in which the temporal behavior of the solution occurs on a much slower scale than the spatial one. Here it is reasonable to use low-order accurate finite difference schemes in order to advance the solution in time. The problem that one faces here is that spectral methods require severe time-step limitations when an explicit time marching technique is applied. In addressing this problem, Gottlieb and Turkel [1980] suggested a second-order in time, unconditionally stable scheme. This scheme seems to perform satisfactorily for Fourier methods but their success in the case of Chebyshev methods is still questionable. For parabolic problems the modification of the DuFort-Frankel scheme was suggested by Gottlieb and Gustafsson [1976], Gottlieb and Lustman [1981], and has been later investigated by Funaro [1983a].

The third class of flow problems involves phenomena in which the temporal and spatial evolution occur on the same scale. It is still possible to use finite differencing techniques for time marching but the time-step must be small. Another alternative is to use spectral discretization in time; however this approach usually leads to a very large and complicated set of equations. Morchoisne [1979] suggested to simplify the set of equations thus obtained by using the idea of approximate factorization. Several other methods are discussed by Deville, et al. [1981].

8.2. Time-stepping Methods for Incompressible Flow Problems

Here, we survey time-stepping methods and boundary condition procedures for incompressible Navier-Stokes equations which are incompletely parabolic and time singular. The equations are

$$\frac{\partial \vec{v}}{\partial t} + \vec{\nabla} p = - \vec{v} \cdot \vec{\nabla} \vec{v} + \nu \nabla^2 \vec{v} + \vec{f} \qquad (\vec{x} \in D), \tag{8.1}$$

$$\vec{\nabla} \cdot \vec{v} = 0 \qquad (\vec{x} \in D), \tag{8.2}$$

where $\vec{v}(\vec{x},t)$ is the velocity field at $\vec{x},t$, $p(\vec{x},t)$ is the pressure, ν is the kinematic viscosity and $\vec{f}(\vec{x},t)$ is an external force. The (constant) density is assumed to be 1. If the boundaries of the region D in which the flow satisfying (8.1) - (8.2) occurs are stationary, then for $\nu > 0$, the appropriate boundary conditions are the no-slip conditions

$$\vec{v}(\vec{x},t) = 0 \qquad (\vec{x} \in \partial D). \tag{8.3}$$

The pressure in (8.1) may be considered a Lagrange multiplier that ensures satisfaction of the (kinematical) incompressibility constraint (8.2) everywhere in D. The most obvious way to obtain an equation for p is to take the divergence of (8.1) and apply (8.2), which gives the Poisson equation

$$\nabla^2 p = - \vec{\nabla} \cdot (\vec{v} \cdot \vec{\nabla}) \vec{v} + \vec{\nabla} \cdot \vec{f} \qquad (\vec{x} \in D). \tag{8.4}$$

A warning of possible trouble in the numerical solution is given when boundary conditions for (8.4) are sought (Orszag and Israeli [1974]). Applying (8.3) to (8.1) gives

$$\dot{\vec{\nabla}} = \nu\nabla^2\vec{v} + \vec{f} \qquad (\vec{x} \in \partial D), \qquad (8.5)$$

so both Dirichlet and Neumann conditions for p are available if $\vec{v}$ is known. In numerical integrations of (8.1) - (8.3), it is not obvious which of these boundary conditions to use.

The ambiguity regarding boundary conditions on p can be avoided if the pressure is eliminated from (8.1) - (8.3). Applying the operator $\vec{\nabla}\times(\vec{\nabla}\times\ldots)$ to (8.1) gives, using (8.2),

$$\frac{\partial}{\partial t}\nabla^2\vec{v} = \vec{\nabla}\times\left(\vec{\nabla}\times(\vec{v}\cdot\vec{\nabla})\vec{v}\right) + \nu\nabla^4\vec{v} - \vec{\nabla}\times(\vec{\nabla}\times\vec{f}) \qquad (\vec{x} \in D). \qquad (8.6)$$

For flow in a plane channel, implicit time-stepping of the linear terms in (8.6) gives a fourth-order equation for the component v of $\vec{v}$ in the direction $\vec{n}$ of the normal to the channel walls. The boundary conditions on v_n are $v_n = \partial v_n/\partial n = 0$. Once v_n is known, the other components of $\vec{v}$ are obtained using incompressibility and the equation for the component of vorticity in the direction $\vec{n}$. The numerical implementation of this scheme is discussed in Appendix II of Orszag and Patera [1983].

A one-dimensional linear model that embodies the essential features of the incompressibility and viscous terms of the Navier-Stokes equations is obtained by considering a solution to the two-dimensional Stokes equations of the form

$$\vec{v} = \left(u(y,t)e^{ikx},\ v(y,t)e^{ikx}\right),\ p = p(y,t)e^{ikx}$$

for some real wavenumber k. Further details of the following analyses are given by Orszag, Israeli and Deville [1983]. The equations satisfied by (u,v,p) are

$$\frac{\partial u}{\partial t} = - ikp + \nu(u_{yy} - k^2 u)$$

$$\frac{\partial v}{\partial t} = - \frac{\partial p}{\partial y} + \nu(v_{yy} - k^2 v) \qquad (8.7)$$

$$iku + \frac{\partial v}{\partial y} = 0,$$

for $-1 \leq y \leq 1$. The boundary conditions are

$$u(\pm 1, t) = v(\pm 1, t) = 0, \qquad (8.8)$$

which simulate rigid no-slip boundary conditions. In general three-dimensional geometries, the equations are coupled and are not easily solved. The solution to an initial-value problem for (8.7) - (8.8) can be expressed in terms of normal modes, for which

$$(u,v,p)\ (y,t) = e^{\bar{\sigma} t}(\hat{u},\hat{v},\hat{p})\ (y), \qquad (8.9)$$

with symmetric modes

$$\hat{v}(y) = \cos \bar{\mu} \cosh ky - \cosh k \cos \bar{\mu} y \qquad (8.10)$$

or antisymmetric modes

$$\hat{v}(y) = \sin \bar{\mu} \sinh ky - \sinh k \sin \bar{\mu}\ y. \qquad (8.11)$$

Here

$$\bar{\mu} = \left(- \frac{\bar{\sigma}}{\nu} - k^2\right)^{1/2} \qquad (8.12)$$

satisfies the eigenvalue relations

$$k \tanh k = -\bar{\mu} \tan \bar{\mu} \tag{8.13}$$

for (8.10) and

$$k \coth k = \bar{\mu} \cot \bar{\mu} \tag{8.14}$$

for (8.11). These eigenmodes are complete on the interval $|y| \leq 1$.

Here we outline several schemes for the solution of (8.7), (8.8) in which time t is discretized by differences but space x is discretized spectrally.

Scheme I: Full Implicit Time Differencing

The system (8.7) - (8.8) is approximated by backwards Euler time differencing:

$$\begin{aligned} \frac{u^{n+1} - u^n}{\Delta t} &= ikp^{n+1} + \nu(D^2 - k^2)u^{n+1} \\ \frac{v^{n+1} - v^n}{\Delta t} &= Dp^{n+1} + \nu(D^2 - k^2)v^{n+1} \\ iku^{n+1} + Dv^{n+1} &= 0, \end{aligned} \tag{8.15}$$

where the superscript index n indicates time level $n\Delta t$ and D indicates a spectral $-y$ derivative. It follows that

$$\frac{1}{\Delta t}(D^2 - k^2)u^{n+1} - \nu(D^2 - k^2)^2 u^{n+1} = -\frac{ik}{\Delta t} Dv^n - \frac{k^2}{\Delta t} u^n, \tag{8.16}$$

with $u^{n+1} = Du^{n+1} = 0$ at $y = \pm 1$. It may be shown that this scheme is stable and spectrally accurate in y and first order in Δt. Methods to solve (8.16) for the spectral representation of u^{n+1} are given in Orszag, Israeli and Deville [1983]. Higher order results in Δt are easily obtained by using higher order time differencing methods.

Scheme II: Implicit Time Splitting

Here the time-differencing scheme involves two split (or fractional) time-steps (Orszag and Kells [1980]). The first steps involves solution of the inviscid equations

$$\frac{u^* - u^n}{\Delta t} = - ikp^*$$

$$\frac{v^* - v^n}{\Delta t} = Dp^* \qquad (8.17)$$

$$iku^* + Dv^* = 0$$

for $|y| < 1$ with boundary condition

$$u^* = 0 \qquad (y = \pm 1).$$

The second step involves the solution of the viscous equations

$$\frac{u^{n+1} - u^*}{\Delta t} = \nu(D^2 - k^2)u^{n+1}$$

$$\frac{v^{n+1} - v^*}{\Delta t} = \nu(D^2 - k^2)v^{n+1}$$

for $|y| < 1$ with boundary conditions

$$u^{n+1} = v^{n+1} = 0 \qquad (y = \pm 1).$$

In this scheme, u^n and v^n do not satisfy the incompressibility constraint (8.2), although the intermediate variables u^* and v^* do. In comparison with Scheme I, Scheme II has the advantage of only involving the solution of

second-order Helmholtz (or Poisson) equations. In general geometries, it offers significant simplifications compared to unsplit schemes. However, Scheme II suffers from large time-stepping errors if $\nu\Delta t$ is large; these can only be removed at considerable computational expense by extrapolation (see Orszag, Israeli and Deville [1983]).

It is by no means obvious that Scheme II has solutions consistent (and convergent) to the solutions of the Stokes equations. For example, it follows from (8.17) and the boundary conditions that

$$Dp^* = 0 \qquad (y = \pm 1),$$

but (8.7) gives

$$Dp = \nu D^2 u \qquad (y = \pm 1),$$

which is, in general, not vanishing. It seems that there is an $O(1)$ error in D_p as $\Delta t \to 0$ at $y = \pm 1$. Nevertheless, Orszag, Israeli and Deville [1983] shows that, away from the boundaries $y = \pm 1$, the global error estimates

$$u^n(y) - u(y,n\Delta t) \sim u_1(y)\Delta t + O(\Delta t^{3/2}) \tag{8.19}$$

$$v^n(y) - v(y,n\Delta t) \sim v_1(y)\Delta t + O(\Delta t^{3/2}) \tag{8.20}$$

$$p^n(y) - p(y,n\Delta t) \sim p_1(y)\Delta t + O(\Delta t^{3/2}), \tag{8.21}$$

hold for fixed y with $|y| < 1$ as $\Delta t \to 0$, where u_1, v_1, p_1 are finite functions of y. Near the boundaries $y = \pm 1$, the error estimates (8.19), (8.20) hold together with

$$Du^n(y) - Du(y,n\Delta t) = O(\Delta t^{1/2})$$

$$D^2 u^n(y) - D^2 u(y,n\Delta t) = O(1)$$

$$D^2 v^n - D^2 v(y,n\Delta t) = O(\Delta t^{1/2})$$

$$p^n(y) - p(y,n\Delta t) = O(\Delta t^{1/2})$$

for $|y| - 1 = O((\nu\Delta t)^{1/2})$, while the error in Dp is, as noted above, $O(1)$ is this region.

Scheme III: Boundary-Divergence-Free Implicit Time Splitting

Marcus, Orszag and Patera [1982] and Marcus [1983] use a modification of Scheme II that removes much of the boundary errors analyzed above. The idea is that splitting error induces large boundary errors because a large divergence of (u,v) develops near the boundaries $|y| = 1$ on the viscous step. The modified method is based on the observation that the normal flow boundary condition $v = 0$ is applied twice each time-step in Scheme II so that by relaxing these conditions on v it may be possible to reduce the error in the boundary divergence. The modified scheme is given by dropping $v^* = 0$ at $y = \pm 1$ in favor of the condition

$$iku^{n+1} + D\,v^{n+1} = 0 \qquad (y = \pm 1), \tag{8.22}$$

while applying (8.17) and (8.18). Thus, normal flow is allowed at the boundary during the inviscid pressure step in order to ensure that (8.22) holds. Analysis of this modified scheme shows that it is uniformly first

order in Δt as a function of y, while higher-order time differencing methods (e.g., Crank-Nicolson differencing) leads to correspondingly higher-order results. However, in more than two space dimensions, large matrix inversions are required by this method.

8.3. Iterative Methods

The system of algebraic equations which results from a pseudospectral approximation to elliptic problems or evolution problems (with implicit time discretization) may be written as

$$L(u) = f \tag{8.23}$$

where L is an operator, possibly nonlinear, f is a known vector, and u is the approximate solution. As shown in Sections 2 and 4, even in the linear case the matrices which represent the operator are full and are difficult to invert directly. Various basic iterative schemes which are available to solve (8.23) can be discussed within the framework of the defect correction procedure. Suppose there is a sparse, efficiently invertible matrix H which approximates the Jacobian J_L of L. Let u^n be a guess for a solution u of (8.23). Taylor expansion about u^n gives

$$\begin{aligned} 0 &= L(u) - f \\ &= L(u^n) - f + J_L(u - u^n) + O\left([u - u^n]^2\right) \\ &\simeq L(u^n) - f + H(u - u^n). \end{aligned}$$

Thus, the simplest defect correction iterative scheme

$$H(u^{n+1}) = H(u^n) - \left[L(u^n) - f\right],$$

or

$$u^{n+1} = u^n - H^{-1}\left[L(u^n) - f\right]. \tag{8.24}$$

The various iterative methods differ in the choice of the preconditioning operator H. For instance, in the case of Jacobi's method, H is the diagonal of J_L, and for the Gauss-Seidel method, H is the lower triangular part of J_L (Hageman and Young [1981]).

Morchoisne [1979] has applied the pseudospectral method in space and time to the unsteady two-dimensional Navier-Stokes equations - in the form of a fourth order equation in the stream function. He used for a preconditioning operator the approximate factorization of the Navier-Stokes operator. More specifically, the operators L and H were defined as in the usual notation with $\Delta \equiv \nabla^2$

$$L(\psi^n) = -\frac{\partial \psi^n}{\partial t} - \frac{\partial \psi^n}{\partial y}\frac{\partial}{\partial x}\Delta\psi^n + \frac{\partial \psi^n}{\partial x}\frac{\partial}{\partial y}\Delta\psi^n + \nu\Delta\Delta\psi^n,$$

with $x,y,t;\ [-1,1] \times [-1,1] \times [0,T]$, and $H \equiv \mathscr{L}_y\,\mathscr{L}_x\,\mathscr{L}_t$ where

$$\mathscr{L}_t = \frac{1}{\varepsilon\eta^\sigma}\left(1 + \varepsilon\frac{\partial}{\partial t}\right)$$

$$\mathscr{L}_x = \left(1 + \varepsilon u^n\frac{\partial}{\partial x} - \varepsilon\nu\frac{\partial^2}{\partial x^2}\right)\left(1 - \eta\frac{\partial^2}{\partial x^2}\right)$$

$$\mathscr{L}_y = \left(1 + \varepsilon v^n\frac{\partial}{\partial y} - \varepsilon\nu\frac{\partial^2}{\partial y^2}\right)\left(1 - \eta\frac{\partial^2}{\partial y^2}\right)$$

and

$$u^n = \frac{\partial \psi^n}{\partial y}, \quad v^n = -\frac{\partial \psi^n}{\partial x}.$$

The nonstationary analogue of the basic iterative scheme (8.24), is the preconditioned Richardson's method

$$u^{n+1} = u^n - \alpha_n H^{-1}[L(u^n) - f], \tag{8.25}$$

which has faster convergence. The convergence rate can further be accelerated by applying polynomial acceleration (Hageman and Young [1981]) to (8.24):

$$u^{n+1} = \omega_n u^n - \alpha_n \omega_n H^{-1}(L(u^n) - f) + (1 - \omega_n)u^{n-1}.$$

This is usually called a nonstationary second degree iterative scheme and it includes Chebyshev and conjugate gradient methods (Hageman and Young [1981]).

Orszag [1980] discusses the Richardson, Chebyshev and conjugate gradient iterative schemes in the linear case, and suggests that the preconditioning operator H should be a suitably chosen, low-order finite-difference approximation H_{FD} to L. For a differential equation dominated by second derivative terms, Orszag [1980] shows that

$$m \leq \| H_{FD}^{-1} L \| \leq M,$$

with $m = 1$ and $M \sim 2.5$. Unfortunately, $\| H_{FD}^{-1} L \|$ is unbounded if L is a first derivative operator and H_{FD}, a central difference approximation. In order to keep $\| H_{FD}^{-1} L \|$ bounded in this case, it is necessary to have more degrees of freedom (grid points) for H_{FD} than for L, and then to modify suitably higher frequencies in the spectral approximation. An alternate remedy is discussed in Hussaini and Zang (this volume) where a semi-implicit Fourier-Chebyshev pseudospectral method of solution (involving a finite

difference preconditioning) is described for solving the unsteady two-dimensional incompressible Navier-Stokes equations.

In multi-dimensional problems it may prove expensive to evaluate the inverse of H_{FD}. Efficiently invertible approximate versions of H_{FD} such as approximate factorizations and incomplete LU decomposition of H_{FD} are the obvious choices. As noted earlier Morchoisne [1979] used approximate factorization for the Navier-Stokes equations. Zang, et al. [1982] and Wong, et al. [1983] discuss several types of LU decompositions. Application of these preconditioning operators is typically far less expensive than the spectral evaluation of the residue. Thus, there is a large payoff for improving the effectiveness of the preconditioning and in using iterative schemes with better convergence rates.

The minimum residual (MR) method (Wong, et al. [1983]) is a robust parameter-free scheme. The only requirement for convergence is that all the eigenvalues of $H^{-1}L$ be strictly in the right half of the complex plane. It can be put in the form of the classical Richardson iterative scheme (8.3) where

$$\alpha_n = \frac{(r^n, Lv^n)}{(Lv^n, Lv^n)}$$

$$r^n = Lu^n - f$$

$$v^n = H^{-1} r^n.$$

Figure 3 shows the convergence history of MR solutions to this Chebyshev pseudospectral approximation to the two-dimensional Poisson's equation with Dirichlet boundary conditions (Wong, et al. [1983]). The labels A and B refer to different LU decompositions; the labe I indicates no preconditioning.

Spectral multigrid methods are very much in the initial stages of development. The work of Zang, et al. [1982] and Hussaini and Zang (this volume) suggests that multigrid procedures which have significantly improved the rates of convergence for finite difference and finite element methods, may do equally well in the case of spectral methods. A glimpse of this promise is seen in Table I which compares the convergence history of Richardson's iteration on a single grid with that of multigrid with Richardson's relaxation for smoothing for Poisson's equation with periodic boundary conditions. Further results are reported in Zang, et al. [1983].

Table I. RMS Residual

Relaxation	Single Grid	Multigrid
3	2.73 (1)	1.82 (7)
6	2.08 (1)	2.42 (-1)
9	1.63 (1)	6.35 (-3)
12	1.31 (1)	4.56 (-4)
15	1.07 (1)	8.30 (-5)

9. INCOMPRESSIBLE FLOWS

9.1 Three-dimensional Numerical Algorithms

The spectral simulation of viscous incompressible (external and internal) flows up to 1974 were reviewed by Orszag and Israeli [1974]. We present here a detailed description of a spectral algorithm for the solution of the Navier-Stokes equations (8.4) in the case of three-dimensional plane shear flows. The physical domain for these flows extends to infinity in the horizontal

directions and is assumed periodic in those directions; in the vertical direction, the flow is either confined between two parallel rigid walls $|y| \leq 1$ (plane channel flow) or bounded by a wall on the one side and extends to infinity in the other direction (boundary layer flow). In this case, it is natural to expand the flow field $\vec{v} = (u,v,w)$ in Fourier series in x and z, and Chebyshev polynomials in y.

$$\vec{v}(\vec{x},t) = \sum_{|k_x|<N_1} \sum_{|k_z|<N_2} \sum_{k=0} \tilde{\vec{v}}(k_x k_z, k, t) e^{i(k_x \alpha x + k_z \beta z)} T_k(y),$$

where $\alpha = \frac{2\pi}{L_1}$, $\beta = \frac{2\pi}{L_2}$, $0 < x < L_1$, $0 < z < L_2$ and $T_k(y)$ denotes the kth degree Chebyshev polynomial. The solution techniques of Orszag and Kells [1980], Moin and Kim [1980] and Kleiser and Schumann (this volume) uses the Adams-Bashforth method for time discretization and are essentially similar except for the different treatment of the incompressibility condition. Orszag and Kells employ a three-level fractional time-step in which the divergence-free condition of the flow field is satisfied at the second fractional step. Moin and Kim solve the continuity equation directly along with the momentum equations. Kleiser and Schumann use an influence matrix technique.

The first fractional step in Orszag and Kells [1980] algorithm is

$$\frac{\hat{\vec{v}}^{n+1} - \vec{v}^{n}}{\Delta t} = \frac{3}{2} F^n - \frac{1}{2} F^{n-1} - \frac{i}{2} k_x \alpha U(y) \left[\hat{\vec{v}}^{n+1} - 2\hat{\vec{v}}^{n} + \hat{\vec{v}}^{n-1}\right],$$

where $U(y)$ is the mean velocity. This results from solving the advection part rewritten as

$$\frac{\partial \vec{v}}{\partial t} + U(y) \frac{\partial \vec{v}}{\partial x} = \vec{F} + U(y) \frac{\partial \vec{v}}{\partial x},$$

by applying the Crank-Nicolson scheme on the left side and Adams-Bashforth

scheme on the right. The nonlinear terms $\vec{F} = (\vec{v} \times \nabla \times \vec{v})$ are computed using the pseudospectral method. No boundary conditions are applied at this stage. The second fractional step consists of

$$\hat{\vec{v}}^{n+1} - \hat{\vec{v}}^{n} = - \Delta t \, \nabla \hat{\pi}^{n+1}$$

$$\nabla \cdot \hat{\vec{v}}^{n+1} = 0,$$

where $\hat{\pi}$ is the total pressure. The impermeability conditions

$$v = 0 \quad \text{at} \quad y = \pm 1$$

are imposed at this stage. The third fractional step includes the viscous effects and the no-slip boundary conditions

$$\vec{v}^{n+1} - \hat{\vec{v}} = \nu \Delta t \cdot \nabla^2 \vec{v}^{n+1}$$

$$\vec{v}^{n+1} = 0 \quad \text{at} \quad y = \pm 1.$$

In summary, this algorithm consists of a spectral tau method with the nonlinear terms computed by pseudospectral method. It has a global error of order $O(\Delta t^2 + \nu \Delta t)$ in time discretization. The time-steps are formally restricted only by the convective limit of the perturbed velocity field.

Moin and Kim [1980] use the Crank-Nicolson method on ∇P and $\nabla^2 \vec{v}$, and Adams-Bashforth on the remaining terms:

$$\nabla^2 \vec{v}^{n+1} - \beta \vec{v}^{n+1} - \frac{1}{2} \nabla P^{n+1} = - \beta \vec{v}^{n} - \frac{1}{2}[3\vec{F}^{n} - \vec{F}^{n-1}] + \frac{1}{2} \nabla P^{n} + \nabla^2 \vec{v}^{n} \equiv \vec{R}^{n},$$

$$\nabla \cdot \vec{v}^{n+1} = 0,$$

where $\beta = \frac{2}{\nu \Delta t}$ and $\vec{F} = \vec{v} \times (\nabla \times \vec{v})$. Fourier transforming the above equations in x and z gives

$$\begin{aligned} \frac{\partial^2 \tilde{\vec{v}}}{\partial y^2} - \left[\lambda + (k_x^2 + k_y^2)\right] \tilde{\vec{v}}^{n+1} - \frac{1}{2} \nabla \tilde{P}^{n+1} &= \tilde{\vec{R}} \\ i\, k_x \tilde{u}^{n+1} + \left(\frac{\partial \tilde{v}}{\partial y}\right)^{n+1} + i k_z \tilde{w}^{n+1} &= 0 \end{aligned} \tag{9.1}$$

where

$$\nabla \tilde{P}^{n+1} = \begin{bmatrix} ik_x \tilde{P}^{n+1} \\ \frac{\partial \tilde{P}^{n}}{\partial y} \\ ik_z \tilde{P}^{n+1} \end{bmatrix} .$$

For every pair of wave numbers k_x and k_z there is a linear system of four ordinary differential equations for u^{n+1}, v^{n+1}, w^{n+1} and P^{n+1}. The y-derivatives in the above system are approximated by either central differences or Chebyshev spectral approximations. Both cases yield a block tridiagonal matrix operator which is inverted by conventional methods.

Although Moin and Kim [1980] discussed an algorithm with Chebyshev polynomials in the vertical direction, all of their published results thus far have used an alternative algorithm which employs finite differences in the vertical direction but retains the Fourier spectral representation in the horizontal direction.

The algorithm of Kleiser and Schumann [1980] differs from that of Moin and Kim [1980] in the solution of equations [9.1). Instead of using the block-tridiagonal matrix inversion method, Kleiser and Schumann (this volume) obtain the solution of this system solving a sequence of one-dimensional scalar Helmholtz equations of the type

$$\frac{\partial^2 \tilde{\vec{v}}}{\partial y^2} - (\lambda + k_x^2 + k_z^2)\, \tilde{\vec{v}} = \vec{b}, \quad \tilde{\vec{v}}(\pm 1) = \tilde{\vec{v}}_1 .$$

Use of the influence matrix technique (Buzbee, et al. [1971]) yields pressure boundary conditions which ensure divergence free solution within round-off errors.

Like Moin and Kim, Wray and Hussaini [1980] also employ central-difference discretization in the vertical direction. However, they address boundary layer rather than channel flow. The boundary layer is assumed to be 'parallel', and a key part of their approach is to treat the mean flow as the solution of the diffusion equation

$$\frac{\partial U}{\partial t} = \nu \frac{\partial^2 U}{\partial y^2}$$

with the Blasius profile as the initial condition. The numerical method is only utilized to calculate the perturbations from this profile. A second major difference is the use of fourth-order Runge-Kutta time discretization. They also satisfy the divergence free condition within round-off errors.

9.2 Application to Hydrodynamic Stability Theory

The eigenvalue problems of hydrodynamic stability theory are often very difficult because they involve the solution of nearly singular boundary value

problems. For example, the solutions to the Orr-Sommerfeld equation that described the stability of plane parallel shear flows typically have boundary layers of thickness $(\alpha R)^{-1/2}$ and an internal layer structure of thickness $(\alpha R)^{-1/3}$, where R is the Reynolds number and α is the streamwise disturbance wavenumber. In this case, spectral methods based on polynomial expansions offer the attractive advantage of high boundary resolution. As discussed by Orszag and Israeli [1974] and Gottlieb and Orszag [1977], only order $1/\sqrt{\delta}$ polynomials are required to resolve a solution with a boundary layer of thickness δ. This property allows the accurate solution of hydrodynamic stability problems with a minimum of spatial degrees of freedom. The general stability analysis code SALLY (Srokowski and Orszag [1977]) is a flexible, accurate code for the analysis of the stability of the boundary layers on aircraft.

The key ideas involved in the generation of modern spectral codes for stability analysis are the use of collocation (pseudospectral) methods, the use of matrix algebra for the setup of the matrix equations to be solved, and the use of the spectral iteration method for the efficient solution of these large matrix equations. The use of matrix algebra is particularly convenient when encountering a new problem for the first time. Here, as we described in Part I, the spectral derivative operators are represented by matrices D, nonconstant coefficient terms are represented by diagonal matrices, and boundary conditions are imposed by replacing suitable rows of the matrix. The resulting scheme for generation of the spectral differential operator is both easy and accurate; it permits the efficient solution of a wide variety of boundary and eigenvalue problems, especially of the kind encountered in hydrodynamic stability theory.

Thus, the pseudospectral matrix representation of the Orr-Sommerfeld equation is simply

$$P\{(D^2 - \alpha^2 I)^2 - iR[(\alpha\bar{U} - \omega)(D^2 - \alpha^2 I) - \alpha \bar{U}''I]\}\phi = 0$$

$$(I - P)B\phi = 0$$

where ϕ is the eigenvector, P is the projection operator onto the interior collocation points (so $I-P$ projects onto the boundary), and B is the operator representing the boundary conditions. The setup of the matrix operator is easily done by algebraic operations applied to the spectral derivative matrix D.

9.3 Applications to Transition and Turbulence

Spectral methods have proven to be the key element in obtaining basic new physical insights in the mechanisms of transition to turbulence. Transition is the process in which a flow first becomes chaotic and random. Because spectral methods are not subject to phase errors, it is possible to use them to follow in detail the nonlinear interaction of waves that would be hopelessly diffused by more conventional finite-difference methods. Several studies of transition phenomena are noteworthy here.

Orszag and Kells [1980] studied the transition to turbulence in plane channel flows and found that one could achieve good agreement with gross experimental features of the flows. In particular, they found that transition typically occurs in plane Poiseuille and plane Couette flows at Reynolds number of the order of 1000, in agreeement with available experimental observations. Their key conclusion, which confirms the experimental

observations of Kovasznay, et al. [1962] and Klebanoff, et al. [1962] and stressed previously by Stuart [1965] and Tani [1969], is the essentially three-dimensional character of transition. In two dimensions, no evidence of real fluid chaos was found.

Wray and Hussaini [1980] studied the transition to turbulence in boundary layers and made comparisons between their numerical flow profiles and available experimental data. In this work, the basic flow was taken as parallel, assuming that the spatial instability of the laboratory boundary layer corresponds to the temporal growth of the numerical boundary layer with periodic boundary conditions. Figure 4 from this work show that the events which constitute the incipient stages of transition (up to the so-called "two-spike" stage) are remarkably similar to the corresponding events observed in the laboratory. A similar set of comparisons between laboratory and numerical experiments has been made for plane Poiseuille flow by Kleiser and Schumann (this volume).

More recently, Orszag and Patera [1981], Pierrehumbert and Widnall [1982], Herbert [1983] and Brachet and Orszag [1983] have used spectral methods to isolate a three-dimensional instability that seems to be primarily responsible for the onset of chaos in shear flows. They have found that the two-dimensional (or axisymmetric) flow states that result from primary, classicial, shear layer instability saturate into ordered finite-amplitude flow states and that, while these finite-amplitude states are stable to two-dimensional disturbances, they are strongly unstable to three-dimensional disturbances. It seems that the three-dimensional flows do not saturate into ordered states and lead directly to chaos.

Marcus, et al. [1982] and Marcus [1983] have made an extensive study of the transition process in circular Couette flow. Marcus [1983] finds that the

onset of wavy Taylor vortex states can be understood in terms of a vortex pairing process, not unlike that encountered in free shear layers and jets. In this work, the flow between rotating cylinders was studied by a high-resolution spectral code using Chebyshev polynomial series in r and Fourier series in θ and z.

There has been a large amouont of research on convecting flows based on the application of spectral methods. The extensive classification of the instabilities of Bernard layers by Busse and his collaborators , has in effect been based on spectral techniques. Busse's pioneering work has clarified both the finite-amplitude stability and roles, and their three-dimensional instabilities. Siggia and Zippelius [1981] have used spectral methods to study the dynamics of defects in Benard convection. McLaughlin and Orszag [1982] used spectral methods to study the onset of chaos in a convecting layer subject to rigid boundary conditions in the vertical direction and periodic boundary conditions in the horizontal. They found substantial agreement with the Ruelle-Takens picture of turbulence in which chaos ensues after three incommensurate frequencies becomes excited. Curry, et al. [1983] made a similar study of the onset of chaos in a convecting layer subject to free-slip boundary conditions on all walls. One of their principal conclusions is that, while two-dimensional convection may be periodic in time, there is as yet no evidence for chaotic motions of the full fluid equations in two dimensions, in contrast to the chaotic motions exhibited by low-order Galerkin (spectral) approximations to the dynamical equations. Goldhirsch and Orszag [1983] have studied the onset theory of chaos in a convecting layer bounded by the three-dimensional rigid walls. In the latter study, three-dimensional Chebyshev expansions are used to resolve the fluid flow.

There are several aspects of these studies of transition that are interesting from the numerical point of view. As mentioned above, Curry, et al. [1983] and Orszag and Kells [1980] find that inadequately resolved two-dimensional flows exhibit spurious time dependence, while adequately resolved two-dimensional flows exhibit much less time dependence than real three-dimensional flows. Toomre, Goughm and Spiegel [1977] found that, provided an adequate amount of vertical resolution was used, spectral models of convection in which a single horizontal mode was retained exhibited no time dependence. Marcus [1981] has found a similar result in a study of convection in spherical geometry; he also found that the threshold for time dependence increases with increasing horizontal resolution.

Another important point concerning numerical simulations of transition is that, in contrast to the turbulence simulations discussed below, transition simulations typically require only modest spatial resolution but extremely high time resolution. It is not uncommon for a transition calculation to require 100,000 or more time-steps, while typical turbulence calculations require at most 1,000 - 10,000 time-steps, even though the latter involve higher resolution spectral codes. The reason is that transition studies often involve relatively weak interactions between modes that require long-time integrations to resolve.

Spectral methods have been used to simulate a variety of turbulent flows. Perhaps the most distinguishing characteristic of high Reynolds number turbulent flows is their large range of excited space and time scales. In homogeneous turbulence, dissipation-scale eddies are of order R times smaller than energy-containing eddies, where R is the Reynolds number. In order to solve the Navier-Stokes equations for such a turbulent flow, it would be necessary to retain $(R^{3/4})$ spatial degrees of freedom and to perform

order $R^{3/4}$ time-steps to calculate for a significant evolution of the flow. Even if only O(1) arithmetic operations were required per degree of freedom per time-step, the total computational work would scale as R^3, while the computer storage requirement would be order $R^{9/4}$. In this case, mere doubling of R requires an order of magnitude improvement in computer capability. In this environment, it may in fact be surprising that significant computations can be performed for turbulent flows; nevertheless, it has been possible to use spectral methods to calculate some key features.

Homogeneous turbulence is simulated by fluid motions within a box with periodic boundary conditions applied. The periodic boundary conditions allow Fourier series representation of the field variables. Starting with the work of Orszag and Patterson [1972], it has been possible to upgrade the spatial resolution of the flows being simulated to the point where it is now possible to simulate flows at Reynolds numbers comparable to those achievable in low-turbulence laboratory experiments. Herring, et al. [1974] and Orszag [976] report simulation of two-dimensional inertial range dynamics, while Brachet, et al. [1983] report the first, albeit crude, calculation of a three-dimensional inertial range spectrum. The work of Brachet, et al. [1983] is based on a numerical simulation of the Taylor-Green vortex, which is a special, highly symmetrical, three-dimensional flow that is a prototype of motions that produce vorticity. With this flow, they were able to achieve an effective spatial resolution of 256 × 256 × 256 Fourier modes for each of the velocity components using the CRAY-1A computer. This allowed enough resolution to obtain a spectrum close to $k^{-5/3}$ where k is the magnitude of the wave number vector, and to obtain the dissipation-fluctuation corrections to this spectrum.

For inhomogeneous turbulent shear flows, Orszag and Patera [1981a or b?], report the first direct numerical simulation of a turbulent channel flow at $R = 5000$ by using a spectral simulation with $64 \times 64 \times 65$ spatial resolution. This calculation was performed by imposing laminar, finite-amplitude two- and three-dimensional Orr-Sommerfeld eigenmodes on an initially laminar velocity profile. They found that, in time evolution, the flow became turbulent and achieved a state consistent with the structure of wall turbulence. In particular, they found that the von Karman "law of the wall" velocity profile was achieved, with a von Karman constant $\kappa = 0.46 \pm 0.05$ (which is good agreement with experiment).

If the resolution of the direct simulation of turbulence is inadequate for the Reynolds numbers that must be simulated, it is possible to use a subgrid scale turbulence closure, called a large eddy simulation, following the pioneering finite-difference work of Deardorff [1970], [1971], [1972] and Schumann [1975]. Here, excitations on scales smaller than those resolvable on the numerical grid are modelled, usually by an eddy viscosity coefficient. Such a sub-grid-scale (SGS) eddy coefficient represents the dissipative effect of motions on scales smaller than the effective grid on the large eddies, (defined as those motions adequately represented on the numerical grid). The most common form for this SGS eddy viscosity coefficient is due to Smagorinsky [1963]

$$\nu_{eddy} = (c\Delta)^2 \left| \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)^2 \right|^{1/2}, \tag{9.2}$$

where Δ is the grid scale and $\vec{v}$ is the large-eddy velocity. In spectral simulations, it is possible to use either (9.2) or some more exotic wave-space filter to remove SGS components. In the absence of walls, either method seems

equally satisfactory. For wall-bounded shear flows, Deardorff calculates only up to the edge of the buffer layer between the viscous sublayer and the logarithmic region of the velocity profile. A boundary condition is imposed at this point based on the von Karman theory of the wall layer in which the turbulent fluctuating stress is assumed known. Molecular viscosity plays no role in Deardorff's calculations, which are performed at least formally, at infinite R. Clearly such a simulation does not give a faithful representation of the wall region and accompanying bursts.

If one is interested in the physics of wall turbulence, neglect of the wall region is unjustified. More recent work by Moin and Kim [1982] integrates up to the rigid wall, the increased sophistication giving a so-called transport eddy simulation. However, the method (as currently implemented) has, in effect, destroyed some of the original incentive of large-eddy simulation. This point is easily demonstrated. As presently practiced, transport-eddy sub-grid-scale simulations use uniform horizontal resolution independent of distance from the wall (Moin and Kim [1982]). If such a simulation is to capture scales down to those of the bursts, the degrees of freedom required scale as R_*^3 where R_* is the wall Reynolds number based on friction velocity. This estimate is based on the fact that streak structure scales with the inner variables (Kline, et al. [1967] and that streamwise and spanwise correlations scale with outer variables, i.e., channel width (Comte-Bellot [1965]). Sub-grid-scale modelling does allow slightly higher Reynolds numbers than those that can be achieved without modelling (Moin and Kim [1982]) achieve $R_* = 640$ by transport-eddy modelling while the direct numerical simulations of Orszag and Patera [1981a] are restricted to $R_* = 200$), but bursts at mean Reynolds numbers of 20,000 - 100,000 (in plane Poiseuille flow) are beyond any sub-grid-scale model as now

implemented. In other words, for a sub-grid-scale, large-eddy simulation to do significantly better than a direct simulation, the dependence of required degrees of freedom must scale less rapidly than R_*^3 as R_* becomes large. At present, no such method exists.

10. COMPRESSIBLE FLOWS

In recent years, spectral methods have begun to be applied to the solution of both steady and time-dependent compressible flow problems. However, in contrast to the sophisticated applications of spectral methods to incompressible flow problems, the applications to compressible flow problems are, to date, less developed.

There are two unique features of compressible flow problems that have required additional theoretical and practical developments in the spectral technique. At first glance, the most difficult problem is that inviscid compressible flows typically develop discontinuous solutions. It is by no means clear that these shocked solutions are amenable to numerical solution by techniques of high formal accuracy like spectral methods. On the one hand, it has been proven (see Section 3), that, for linear problems, high accuracy can be maintained within spectral methods far away from a discontinuity; on the other hand, it may be thought that for nonlinear problems the overall accuracy in the presence of discontinuities is limited to first order. However, Lax [1978] has argued that more information about the solution is contained within high resolution schemes, which may be usefully extracted in obtaining high resolution results.

The other major problem with compressible flows is associated with the boundary conditions that must be applied. For inviscid problems that are

hyperbolic in nature, the analytic solution is driven by the data entering at inflow boundaries and the numerical technique should minimize the influence of conditions imposed on outflow boundaries. Because of the high accuracy of spectral methods and their global nature, correct implementation of boundary conditions is crucial to obtaining stable and accurate results.

10.1 One-Dimensional and Quasi-One-Dimensional Flows

Gottlieb, Lustman and Orszag [1981] considered the solution of one-dimensional, inviscid, compressible flows with shocks by spectral methods. In particular they discussed methods capable of capturing a shock wave over one grid interval. In addition to the conventional shock tube problem, they treated the problem of a strong shock wave overtaking a weak shock resulting in a single shock and a rarefaction wave. To demonstrate resolution of this shock and the contact discontinuity over a single grid interval, the density plot after shock coalescence is reproduced in Figure 5. Figure 5a shows the density distribution after the application of the stabilizing low-pass filter which consists of an exponential cut-off of high frequencies (see Gottlieb, Lustman and Orszag [1981] for details). Figure 5b displays the density distribution after applying what is called the post-processing filter (Gottlieb, Lustman and Orszag [1981]) which is simply three-point averaging except in the immediate neighborhood of the discontinuity itself where the averaging is one-sided.

These simple filters appear to be sufficient to stabilize the solution, suppress the Gibb's phenomenon and possibly achieve spectral accuracy for flow problems consisting of piecewise linear profiles. It remains to be seen if spectral accuracy can be maintained for more structured flows. It should also be noted that in this method, although shock waves are not fitted as

discontinuities, the post-processing filters employed do require knowledge of the shock locations which can be obtained in either physical or spectral space. Even assuming knowledge of the shock locations, there is a serious need for development of spectral filtering techniques to remove with global oscillations without loss of spectral accuracy.

Zang and Hussaini [1980] present pseudospectral solutions to more complicated flow problems. Their results show that a highly structured flow field is well represented along with the sharp front of the shock (see Figure 6). However, the rate of convergence to the inviscid solution is only finite. Other spectral work on one-dimensional shock problems has been done by Taylor, et al. [1981] and Cornille [1982].

10.2 Two-Dimensional Flows

10.2.1 Euler Equations

Gottlieb, Lustman, and Street (this volume) study simple variants of the problem of a regular reflection of an oblique shock wave from a solid surface by solving the Euler equations in conservation form. The pseudospectral technique employed is a straight-forward extension of the method developed for the one-dimensional case (Gottlieb, Lustman and Orszag [1981]). The smoothing and filtering methods which work well in the one-dimensional shock tube problem yield similar results in the two-dimensional shock reflection problem if the flow involved is piecewise uniform.

A careful treatment of the boundary conditions is extremely important as the spectral method is not as forgiving as the finite difference method in this aspect. Imposition of the boundary conditions in the characteristic form is found to work satisfactorily as predicted by the linear theory of Section 6. Figure 7 shows the results of calculations described in Salas, et al.

[1982] for the interaction of a Mach 1.3 shock wave with an idealized Karman vortex street, and it illustrates the sensitivity of spectral methods to boundary treatment. The only difference between the two calculations is the treatment of the left subsonic inflow boundary. For the calculations shown in the top row, all the variables were prescribed. This overspecification of boundary conditions leads to the eventual contamination of the entire solution. In the second calculation, only three of the four variables were specified at the left boundary. The remaining variable, the pressure, was computed from the interior solution along a linearized characteristic. The details of method to impose the boundary conditions is given in Gottlieb, et al. (this volume).

It should be emphasized that spectral methods for even slightly complex discontinuous two-dimensional flows governed by the Euler conditions require further development. To date the best pseudospectral Euler solutions with shock capturing have been obtained for one-dimensional and quasi-one-dimensional flows; as was pointed out in Section 10.1, the post-processing filter did involve explicitly locating the shock, and even so the accuracy of the structured, smooth regions of the flow was affected. Pending development of improved filtering techniques, it is expedient to fit the shock, and thus to maintain the usual advantages that arise from the application of spectral methods to smooth problems.

10.2.2 Shock Fitting

Fitting or tracking a shock in one dimension is simple. It involves a straightforward application of Rankine-Hugoniot conditions. In two dimensions, shock fitting is more complicated. Usually a coordinate transformation is employed so that the shock wave becomes a coordinate

boundary. To be specific, let $x_L \leq x \leq x_s$ $-\infty \leq y \leq \infty$ (see Figure 8) be the region fo computation bounded on the right by the shock wave

$$x = x_s(y,t).$$

Define the coordinate transformation

$$X = \frac{x - x_L}{x_s(y,t) - x_L}, \qquad Y = y, \; T = t$$

where (x,y) is the Cartesian coordinate system in the physical space and t, the physical time. With the flow field in front of the shock known, the flow field immediately behind the shock can be evaluated via the Rankin-Hugoniot conditions if the shock velocity is known.

Let the shock speed be defined by

$$\dot{x}_s = \frac{\partial x_s}{\partial T},$$

and the unit normal $\hat{N}$ to the shock by

$$\hat{N} = \hat{\alpha x} + \hat{\beta y}$$

where $\hat{x}$ and $\hat{y}$ are unit vectors in the x- and y-direction respectively. Then the shock velocity is

$$\vec{\dot{x}}_s = \dot{x}_s \hat{x},$$

and its component in the direction $\hat{N}$ is

$$w_s = \dot{\vec{x}} \cdot \hat{N}.$$

If the velocity field in front of the shock is

$$V = u\hat{x} + v\hat{y},$$

the velocity component relative to the shock in the direction of the normal $\hat{N}$ is

$$\tilde{U}_{rel} = \vec{V} \cdot \hat{N} - w_s,$$

$$= u\alpha + v\beta - w_s,$$

and the Mach number relative to the shock is

$$M_{rel} = \frac{\tilde{U}_{rel}}{a}$$

where a is the sound speed in front of the shock. With the relative Mach number known, the flow variables behind the shock can be evaluated using the Rankine-Hugoniot relations. Then the compatibility relation for the characteristic reaching the shock wave in the x,T plane from the high pressure side is obtained by combining the equation of continuity and the x-momentum equation. If the time derivatives appearing in this expression are replaced by those obtained by differentiating the Rankine-Hugoniot relations $\dot{\vec{x}}$ with respect to T, the equation for shock acceleration $\partial \dot{x}_s / \partial T$ is found. The required shock speed is obtained by integrating this equation.

While solving the equations of motion by explicit time discretization, the shock velocity and position is computed at every step. It should be noted

that the shock boundary in the computational domain is a supersonic inflow boundary, and the Rankine-Hugoniot relations provide the boundary conditions for all of the variables once the unknown shock velocity is computed. The shock fitting strategy described here has been used with the pseudospectral method to study the classical blunt body problem, (Hussaini and Zang (this volume)) and the more complex problem of a shock wave interacting with turbulences (Zang, Kopriva and Hussaini [1983]).

10.2.3 Potential Equations

It is well known that, even with weak shocks, a good approximation to transonic flows is obtained using the compressible potential equation. The most distinguishing and also difficult feature of transonic flows is their mixed subsonic-supersonic character, which was treated computationally by Murman and Cole [1971], who introduced type dependent differencing schemes for steady plane transonic flow.

The extension of type-dependent schemes to use pseudospectral methods applied to transonic potential flow past a parabolic arc are reported in Gottlieb, Lustman, and Streett (this volume). Streett [1983] has obtained pseudospectral solutions for arbitrary lifting airfoils. The airfoil is mapped onto a cylinder using conformal mapping. The full potential equations in the computational plane are solved using the cylindrical polar coordinate system with Fourier representation in the aximuthal direction and Chebyshev polynomial representation in the radial direction. Shocks are captured using the second order artificial density method as in the finite difference codes. For supercritical cases, an iterative scheme combining AF1 (Douglas-Gunn) and AF2, (see Holst [1979]), is found to be fairly efficient. For subcritical flows, four decimal place accuracy in surface pressure and lift is obtained

with a grid of 12 × 40 points, and a typical calculation requires about 45 seconds on CDC CYBER 175. The well known finite difference multigrid code, FLO-36 (Jameson [1979]) requires about 40 seconds on the same computer on a 32 ×192 grid for the same accuracy. The supercritical cases require more resolution and the iterative scheme suffers from slow convergence.

The multigrid procedure given in Streett, et al. [1983] is found to accelerate substantially the convergence rate both in the subcritical and supercritical cases. For example, converged solutions for subcritical flow conditions are obtained in less than 15 seconds on the CYBER 175, using a grid of 16 × 32 points. Even more dramatic improvements are obtained in the case of supercritical flow (Figure 9) where the machine time is reduced by a factor between 20 and 50 over a single grid iteration scheme.

In summary, the iterative schemes developed for finite difference discretization can equally be applied equally well to spectral discretizations. Since the residual calculation is an order of magnitude more expensive than the approximate factorization or approximate inverse calculation, reducing the number of iterations required for a given convergence criterion is the major requirement for a good spectral method.

The artificial density technique using finite differences yields satisfactory results. However, from the standpoint of accuracy, this technique for capturing shocks requires improvement. The advantage of a reduced number of points for a given accuracy is offset by the greater cost per point of the spectral method to the extent that the total cost of a spectral solution may be of the same order as that for the finite difference solution. Improvements in iterative methods, like the multigrid method, promise to give spectral methods that are more efficient in both storage and work than the best available finite difference methods.

10.3 Three-Dimensional Flows

Lambiotte, et al. [1982] have developed a three level time-split spectral/finite difference method for the numerical solution of the three-dimensional compressible Navier-Stokes equations. The first fractional step includes the effect of the advection terms, using a variable-step second-order Adams-Bashforth method. The pseudospectral method is used for calculating x- and y-derivatives. The second fractional step is an implicit pressure correction to avoid numerical instabilities due to sound waves. In the third fractional step, viscous corrections are made to the inviscid solution obtained in the previous two steps. Use of the pseudospectral technique for the evaluation of the compressible viscous terms involve a large amount of computation. Since viscosity is small at large Reynolds number, it is reasonable to limit the computational work by discretizing the viscous terms using central differences. The truncation error is on the order of $\nu(\Delta t + \Delta x^2 + \Delta y^2 + \Delta z^2)$ here ν is the maximum kinematic viscosity. To avoid severe time-step restrictions resulting from small z in the stretched z-mesh, the z-derivatives are treated implicitly. This algorithm is being used to study compressible shear flows at high Reynolds number such as the incipient stages of transition to turbulence, and receptivity of laminar boundary layers to external disturbances.

Feiereisen, Reynolds, and Ferziger [1981] have carried out a numerical simulation of low Reynolds number homogeneous turbulent shear flow using the three-dimensional compressible Navier-Stokes equations. Following Rogallo [1977], they apply a coordinate transformation to the Navier-Stokes equations which permits imposition of periodic boundary conditions. Thus they were able to use a pseudospectral Fourier method in space.

APPENDIX A

The error bounds presented in Sections 3 and 5 for the pseudospectral methods were all derived using energy estimates which are global in space. Consequently, special features of the local behavior of the error may be lost in this analysis.

In an unpublished paper, Dubiner [1977] gave a detailed asymptotic analysis, independent of the energy method, of the error in various spectral methods. His original method is reviewed here for the particular example of the wave equation.

Consider the equation

$$\begin{aligned} u_t &= u_x \qquad |x| < 1 \\ u(x,0) &= f(x) \\ u(1,t) &= q(t). \end{aligned} \tag{A1}$$

Let u_N be the polynomial approximation to the solution u of (A1). This approximation may be obtained either by the pseudospectral, Galerkin or tau Cheyshev methods. In all the above cases u_N satisfies the following equation

$$\begin{aligned} \frac{\partial u_N}{\partial t}(x,t) &= \frac{\partial u_N}{\partial x}(x,t) + \tau_N(t)\, q_N(x) \\ u_N(x,0) &= P_N f = f_N(x) \\ u_N(1,t) &= g(t), \end{aligned} \tag{A2}$$

where $q_N(x)$ is a polynomial of degree N in x and τ_N is a function of t.

In the case of the pseudospectral Chebyshev method based on the collocation points x_j given in (4.1),

$$q_N(x) = \frac{(1+x)T_N'}{2N^2} \; ; \tag{A3}$$

For the pseudospectral method based on the points y_j given in (4.18)

$$q_N(x) = \frac{T_{N+1}'}{N^2} \; , \tag{A4}$$

while for the Galerkin method

$$q_N(x) = \sum_{k=1}^{N} T_k(x) + \frac{1}{2} \tag{A5}$$

and for the tau method

$$q_N(x) = T_N(x) \tag{A6}$$

(Gottlieb and Orszag [1977]). In all cases $\tau_N(t)$ is determined by the condition that $u_N(x,t)$ be a polynomial in x of degree at most N. The quality of the approximation depends on the behavior of the unknown function $\tau_N(t)$. The basic idea of Dubiner's method is to find an expression for $\tau_N(t)$ in terms of $q_N(x)$, $P_N f(x)$ and $g(t)$ using only the fact that u_N is a polynomial in x.

To do this we Laplace transform equation (A2) with respect to time to get

$$s\,\hat{u}_N(x,s) - f_N(x) = \frac{\partial \hat{u}_N(x,s)}{\partial x} + \hat{\tau}_N(s)\, q_N(x) \tag{A7}$$

$$\hat{u}_N(1,s) = \hat{g}(s)$$

where $u_N(x,s)$ is the Laplace transform of $u_N(x,t)$. Equation (A7) is an ordinary differential equation with solution

$$\hat{u}_N(x,s) = e^{s(x-1)}\{\hat{g}(s) + \hat{\tau}(s) \int_1^x e^{-s(\xi-1)} q_N(\xi)\, d\xi - \int_1^x e^{-s(\xi-1)} f_N(\xi) d\xi\}. \quad (A8)$$

Observe now that the left side of (A8) is a polynomial in x, whereas the first term on the right side is growing exponentially with increasing x. Therefore, as $x \to \infty$ the term in the brackets appearing in the right side of (A8) must vanish giving

$$\hat{\tau}_N(s) \int_1^\infty e^{-s(\xi-1)} q_N(\xi) d\xi = -\int_1^\infty e^{-s(\xi-1)} f_N(\xi) d\xi + \hat{g}(s). \quad (A9)$$

Equation (A9) yields the desired expression for the function $\hat{\tau}_N(s)$ that governs the behavior of the error in the spectral approximation to the wave equation.

Dubiner proceeds by considering a large class of polynomials $q_N(x)$ rather than the particular forms (A3) - (A6). This class is characterizied as follows.

Let

$$Z(x) = x\left[1 + \sqrt{1-x^{-2}}\right]$$

and $D(Z)$ be an analytic function (except for algebraic singularities at $x = \pm 1$) that grows less than exponentially fast near infinity. Moreover assume that

$$D(Z) \sim \begin{cases} (1+Z)^{\alpha+1/2} & |Z+1| \ll 1 \\ C_p(1-Z)^{\beta+1/2} & |Z-1| \ll 1 \end{cases}$$

Then we consider the class of polynomials satisfying

$$(2\pi)^{-1/2}\left[D^{-1}(Z^{-1}(x))Z^{N}(x)+D^{-1}(Z(x))Z^{-N}(x)\right] \qquad |x\pm 1| \gg N^{-2/3} \tag{A10}$$

$$P_N\, q_N(x) \sim \quad N^{\alpha+1/2}\ (-1)^N\left(N\sqrt{1-x^2}\right)^{-\alpha}\ J_\alpha\left(N\sqrt{1-x^2}\right) \qquad |x+1| \ll N^{-2/3} \tag{A11}$$

$$N^{\beta+1/2}\ C_p\left(N\sqrt{1-x^2}\right)^{-\beta}\ J_\beta\left(N\sqrt{1-x^2}\right) \qquad |x-1| \ll N^{-2/3}. \tag{A12}$$

This assumption is satisfied by all the orthogonal polynomials with weight function $a(x)$

$$a(x) = (1+x)^{\alpha}\,(1-x)^{\beta}\,b(x), \tag{A13}$$

where $b(x)$ is a nonnegative polynomial on $[-1,1]$, and in particular for the polynomials given by (A3) - (A6).

For this review we omit now the (very sophisticated) asymptotic expansions that lead to the error estimates. In Figure 10 the error of the pseudospectral Chebyshev approximation to $u_t + u_x = 0$ with data which has ℓ smooth derivatives is given. Observe the different behavior in different regions in the x,t plane, a behavior that can not be obtained easliy by the analysis based on energy methods.

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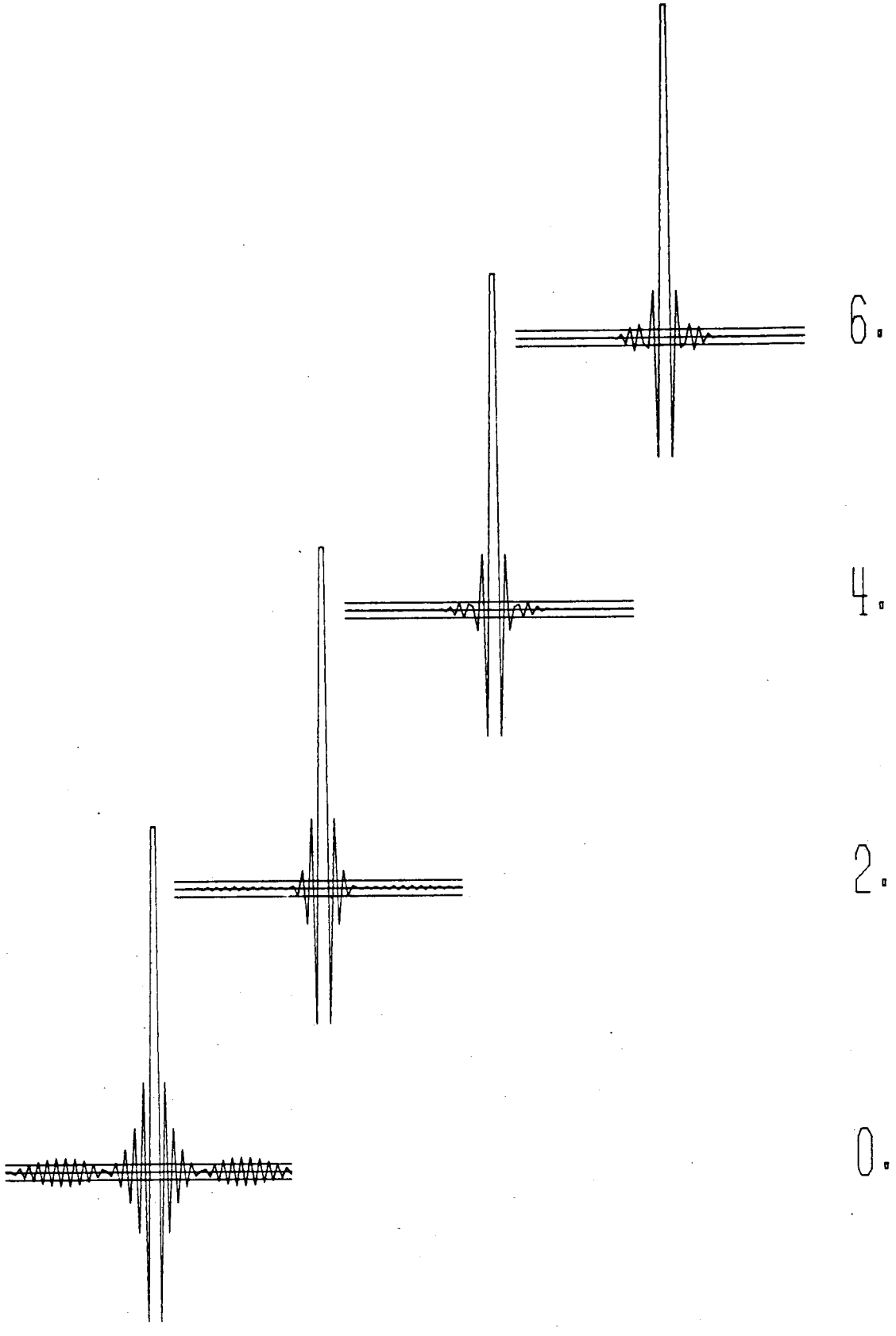


Figure 1. Filtered Fourier derivative of the function

$$u(x) = \begin{cases} x, & 0 \leqq x \leqq \pi, \\ x - 2\pi, & \pi < \leqq 2\pi, \end{cases}$$

with $K_0 = 45$, $N_2 64$, $\rho = 0,2,4,$ and 6 (formula (2.12)).

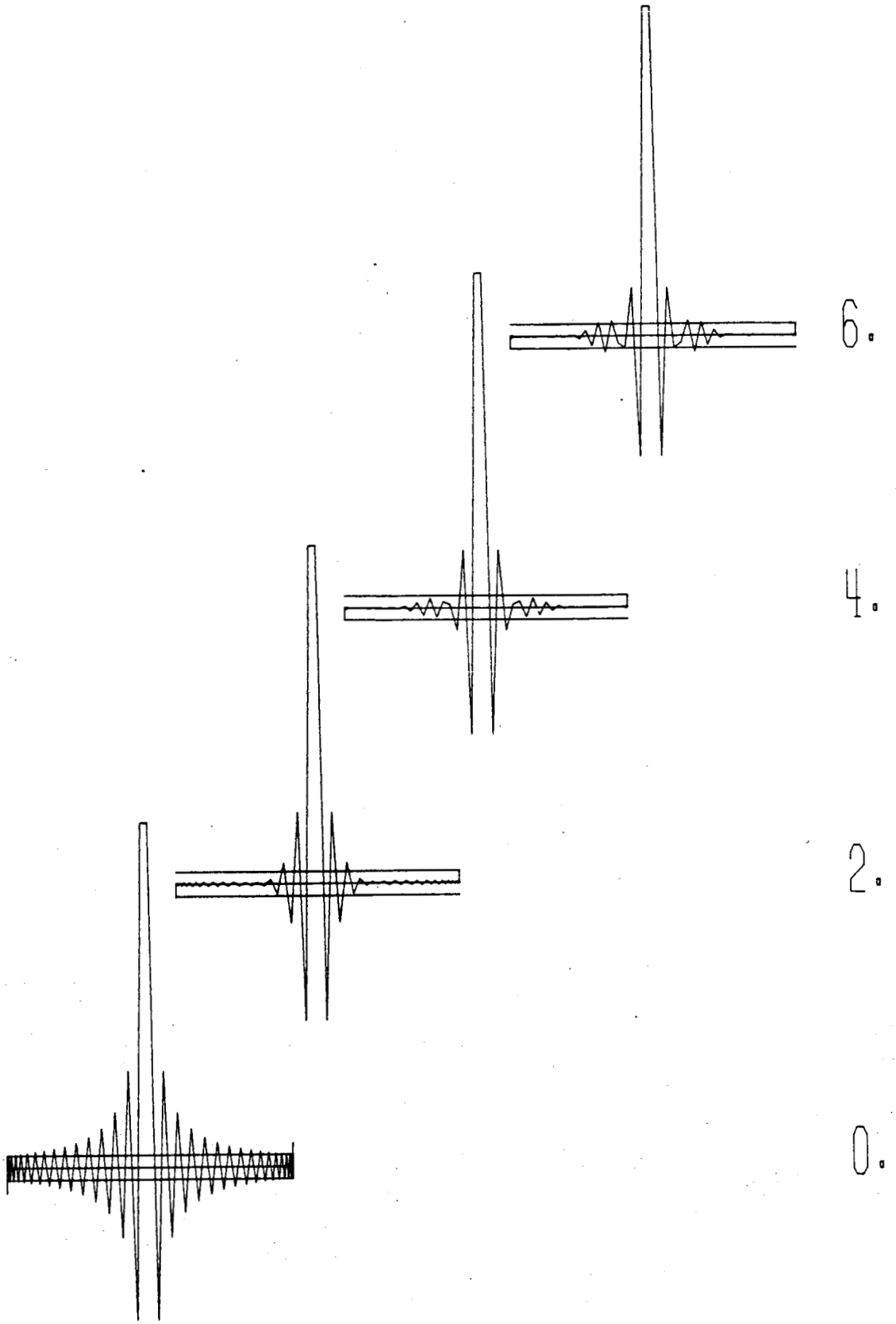


Figure 2. Filtered Chebyshev derivative of a step function with $a_0 = 45$, $N = 64$, $\rho = 0,2,4,$ and 6 (formula (5.8)).

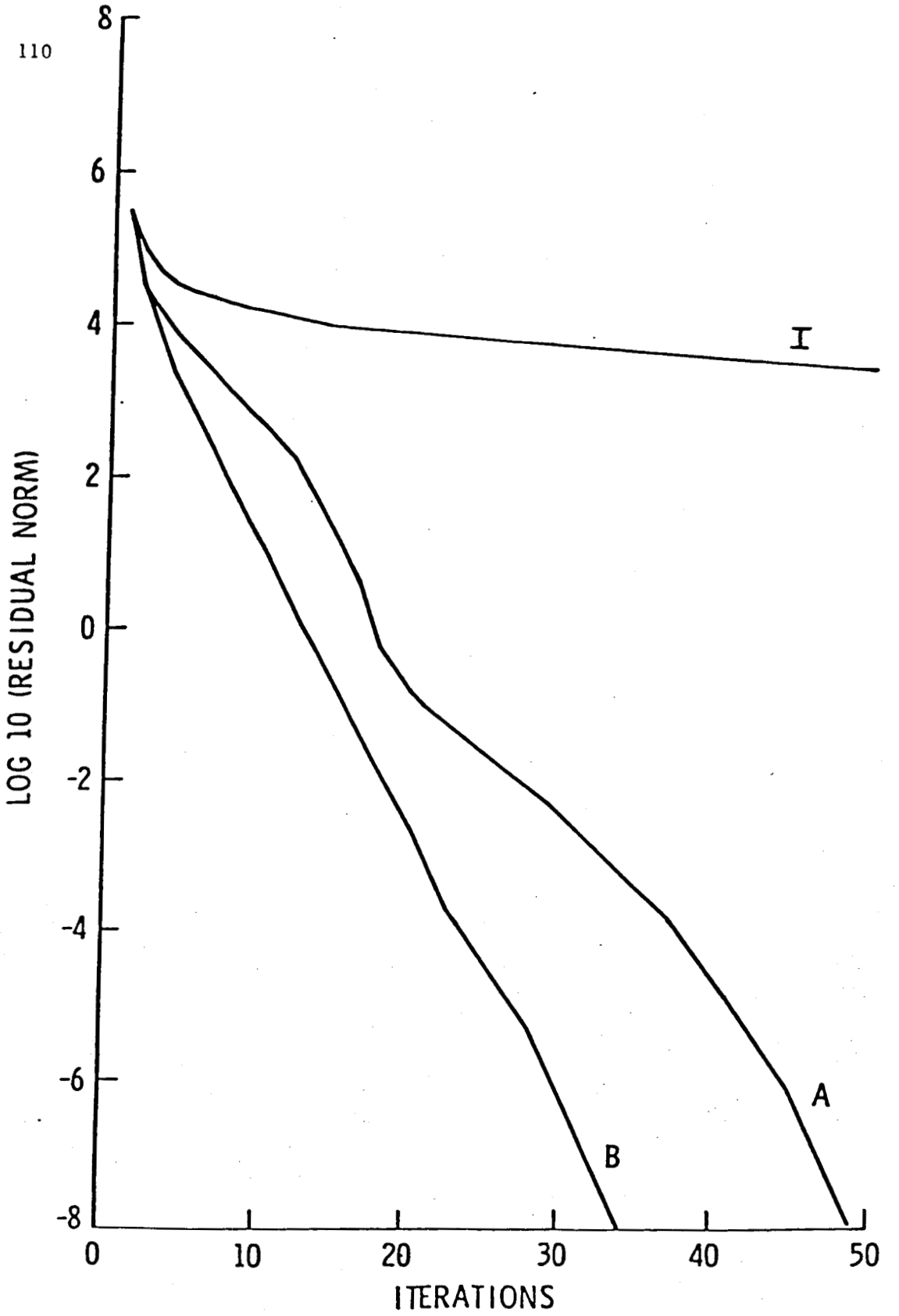
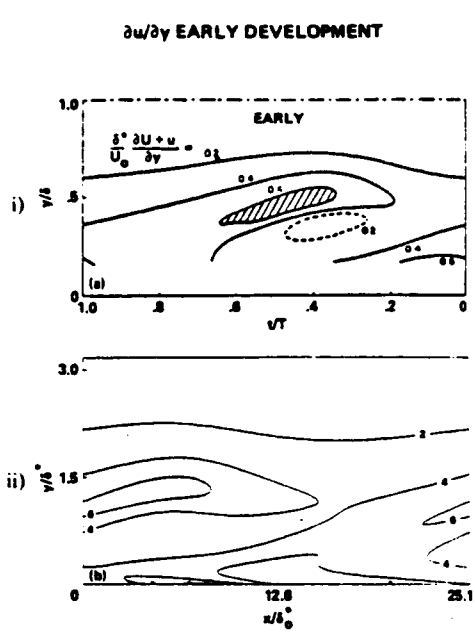
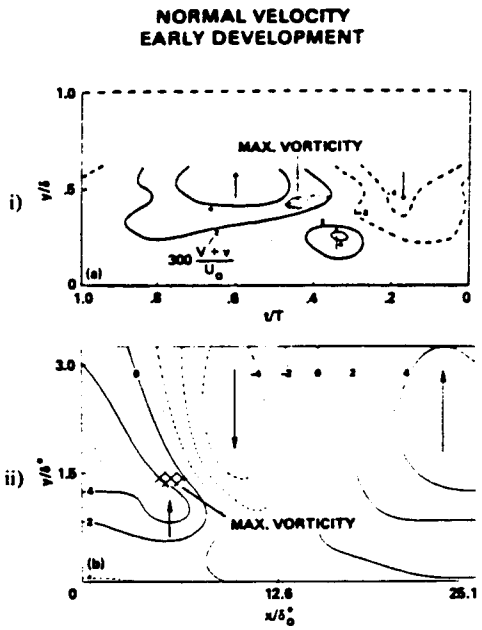


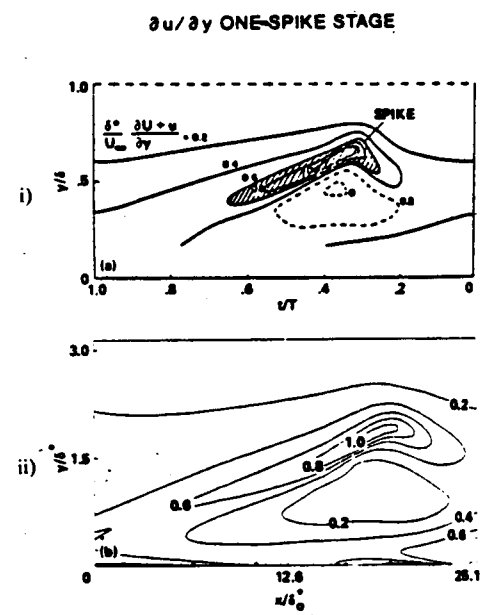
Figure 3. MR method on a 32 × 32 grid.



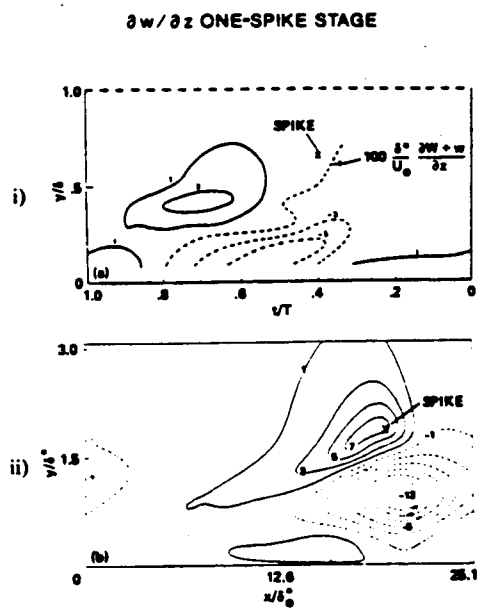
a) *Contours of ∂u/∂y at peak position; early development.* i) *Kovasznay et al.* [73, Fig. 10a]. ii) *Numerical simulation.*



b) *Velocity normal to plate at peak position; early development.* i) *Kovasznay et al.* [73, Fig. 13a]. ii) *Numerical simulation.*



c) *Contours of ∂u/∂y at peak position; one-spike stage.* i) *Kovasznay et al.* [73, Fig. 10b]. ii) *Numerical simulation.*



d) *Lateral vortex stretching rate at peak position; one-spike stage.* i) *Kovasznay et al.* [73, Fig. 12b]. ii) *Numerical simulation.*

Figure 4.

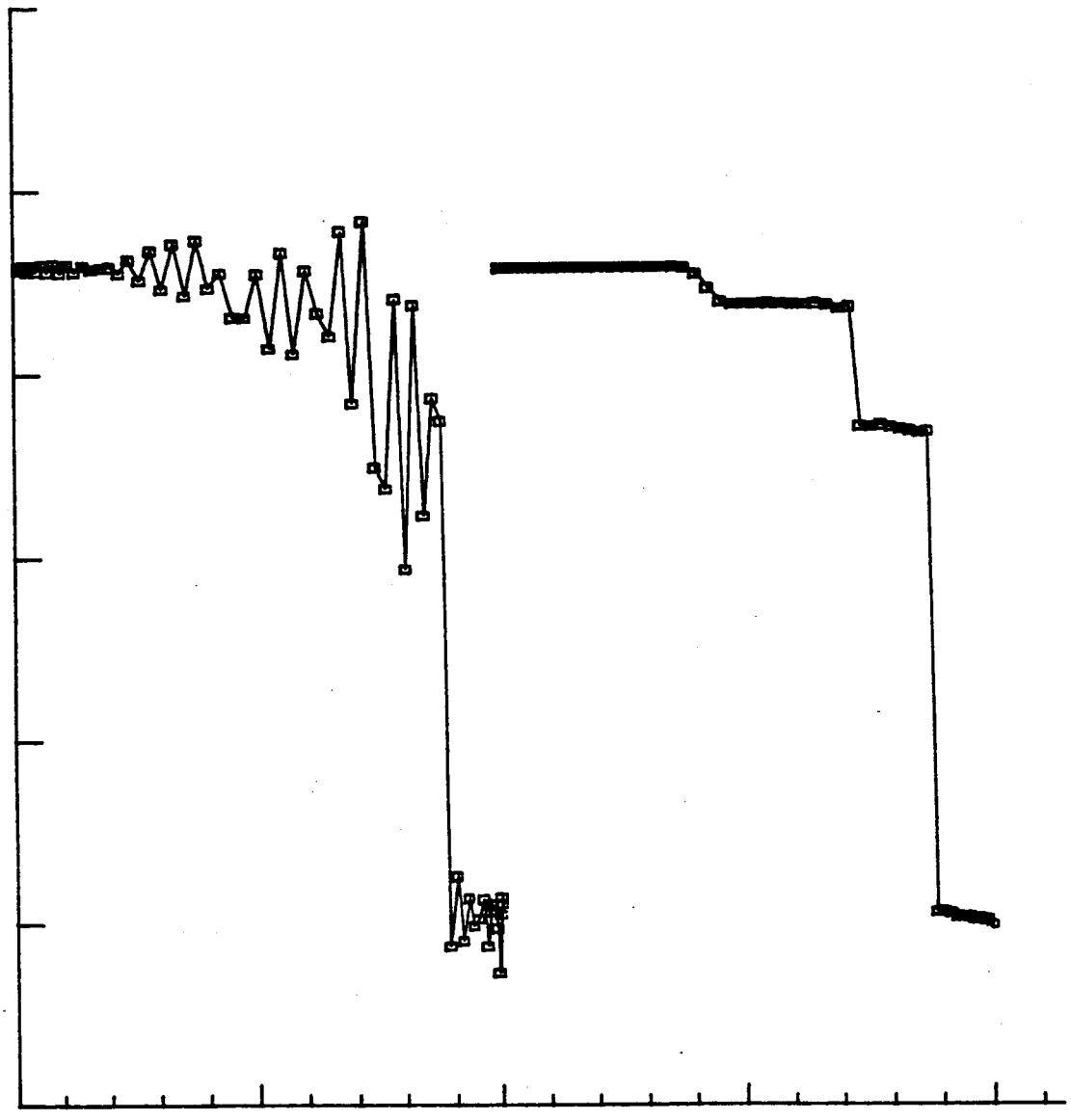
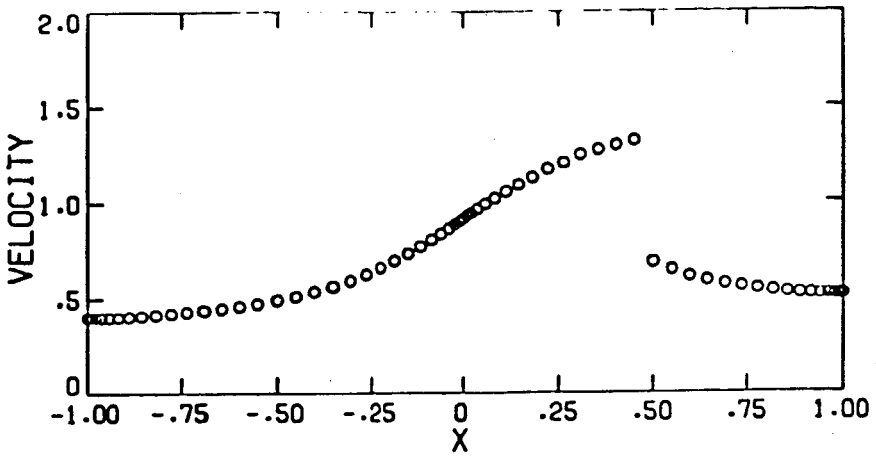
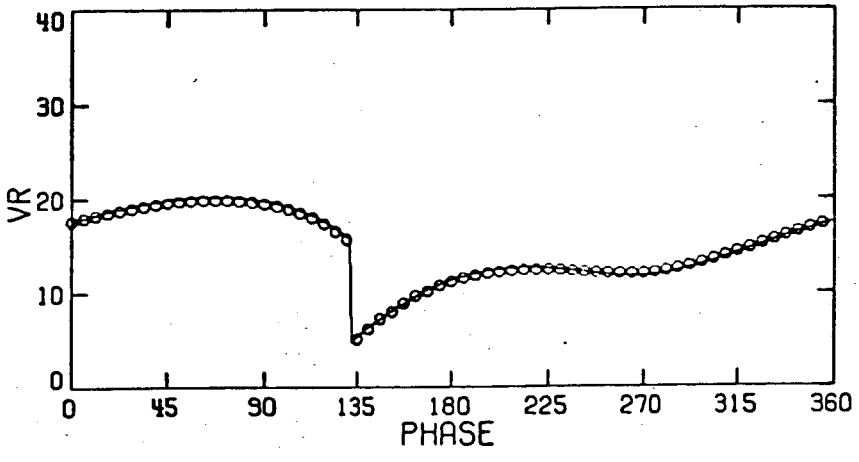


Figure 5. Spectral capturing of shock coalescence without and with post-processing.



Quasi-one-dimensional Nozzle Flow

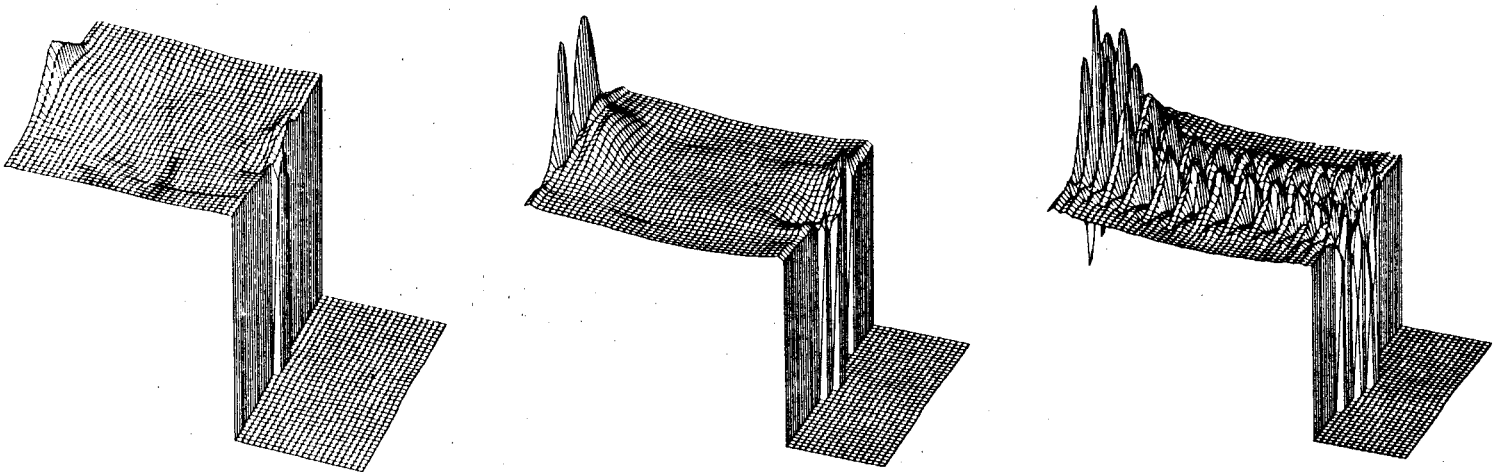


Astrophysical Problem

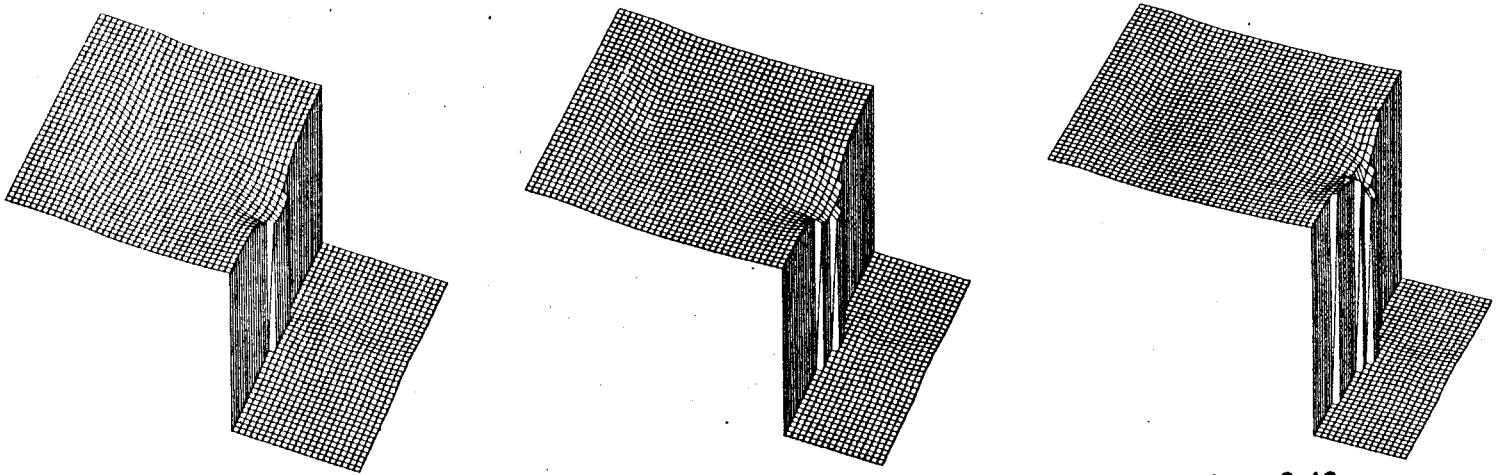
Figure 6

PSEUDOSPECTRAL PRESSURE FOR MACH 1.3 KARMAN VORTEX STREET

OVERSPECIFIED INFLOW CONDITIONS



CHARACTERISTIC INFLOW CONDITIONS



t = 0.29 t = 0.37 t = 0.40

Figure 7

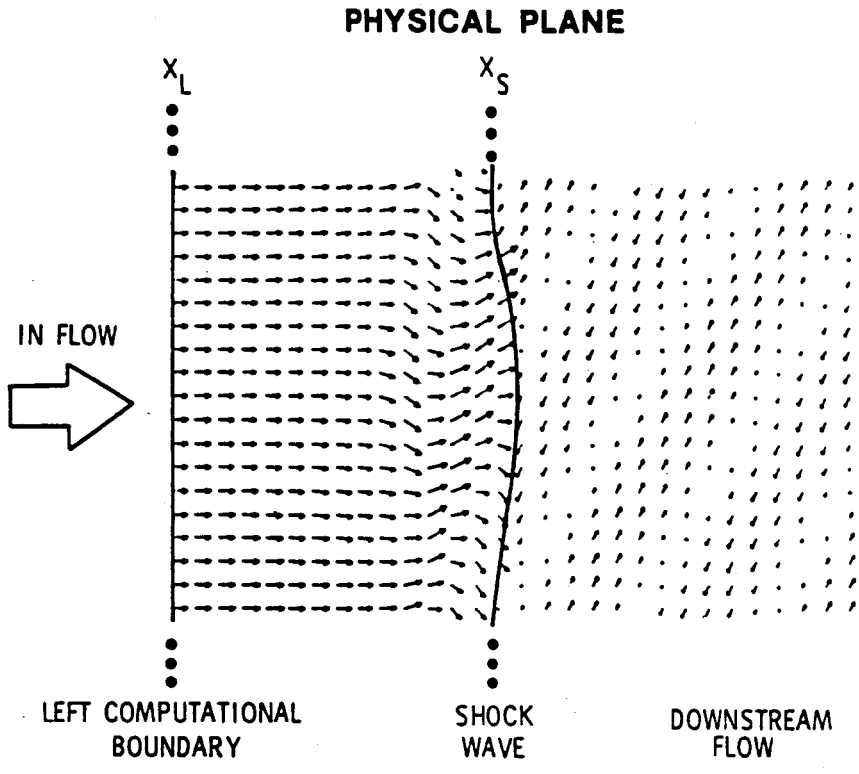

PHYSICAL PLANE
X_L
X_S
IN FLOW
LEFT COMPUTATIONAL BOUNDARY
SHOCK WAVE
DOWNSTREAM FLOW

Figure 8

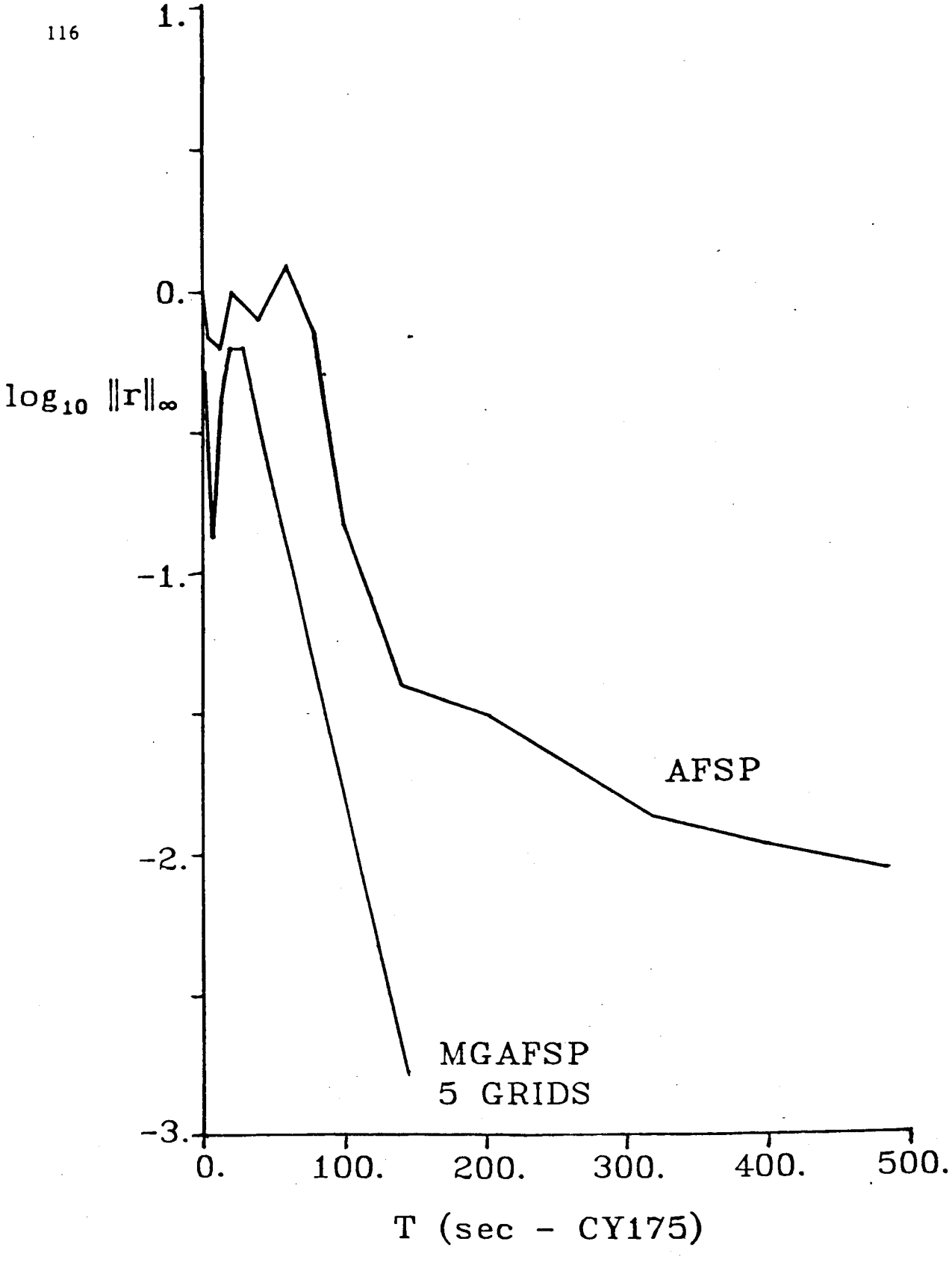


Figure 9. Residual versus machine time.

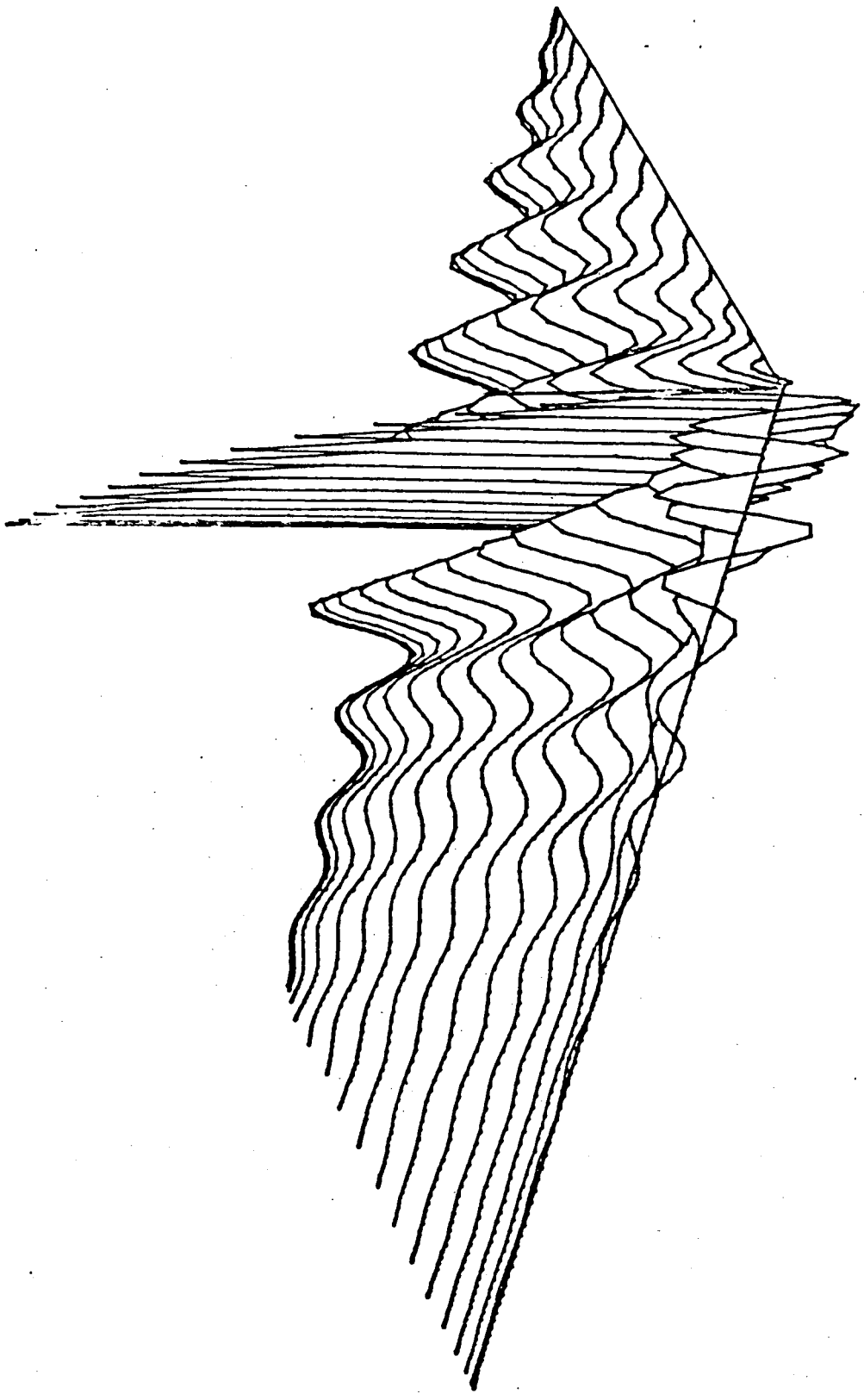


Figure 10. Errors in Chebyshev collocation approximations to $u_t + u_x = 0$.